

# Exploring QSAR

## Hydrophobic, Electronic, and Steric Constants

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**A**LBERT LEO was born in 1925 in Winfield, Illinois, and educated in southern California. He spent two years in the U.S. Army Infantry, serving in the ETO from 1944 to 1945. He received his B.S. in chemistry from Pomona College (1948; Phi Beta Kappa, Magna Cum Laude) and M.S. and Ph.D. in physical organic chemistry from the University of Chicago, studying reaction kinetics under Frank Westheimer. After 15 years in industrial research and development in food chemistry, he returned to Pomona College to initiate and direct the MedChem Project under the leadership of his former professor Corwin Hansch. The project provides software and databases useful in the design of bioactive chemicals and is distributed worldwide. Leo was given an Excellence in Science award by Sigma Xi in 1980 and was chairman of the Gordon Conference on QSAR in Biology in 1981.

**D**AVID HOEKMAN was born in 1961 in Holland, Michigan. He attended Pomona College for five years starting in 1980 and initially majored in physics. After three years of study he switched to biology and received his B.S. in biology in 1985. He spent a year working on ecological wood anatomy with Sherwin Carlquist at Rancho Santa Ana Botanic Garden. After a year of study in the botany department at the University of California at Berkeley, he turned his attentions toward computer programming. Since 1987 he has been the head of computer operations at the MedChem Project, where he designed and implemented a QSAR database and analysis package.

# Contents

Preface	ix
Dedication	xiii
How To Use the Tables in this Volume	xv
■ Octanol LogP	1
■ Octanol LogP Footnotes	194
■ Hammett Sigmas	217
■ Hammett Sigmas Footnotes	305
■ Depiction of Solute Structures	325

# Preface

The motivations for this book are to provide an introduction to what is commonly referred to as "quantitative structure-activity relationships" (QSAR) and to provide substituent constants for their construction. As straightforward as this might sound, it is now virtually an impossible task. There are so many ways to approach the problem, so many computer programs, so many different types of parameters, that no small group can hope to attain a mastery of all of the various methodologies. QSAR is a highly active area of research in which many companies already offer software of all kinds. Thus, this field is often referred to as "computer-assisted drug design" or CADD.

For good reasons, science has been divided into major disciplines, and these disciplines have been divided into innumerable compartments and subcompartments. The subject we are attempting to present resides in a number of major divisions: chemistry, biology, medicine, statistics, computer science, and environmental science. These divisions break down into many large, highly complex, and fast-changing compartments. For example, some of the essential chemical compartments are physical organic, biological, medicinal, quantum, and computational chemistry. Some examples under the heading of biology are molecular, cell, whole animal biology, neurobiology, and psychobiology. Under medicine, there are the diverse areas of chemotherapy, pharmacology, metabolism, and epidemiology. In the computational area, there are the compartments of molecular mechanics and dynamics, pattern recognition, statistics, and database management. Environmental science is concerned with bioconcentration, the distribution of chemicals in various ecosystems as well as toxicology. All of these various specialties play a role in an as yet undefined science: that of how chemicals react with the vast number of forms of life ranging from viruses to bacteria, plants, insects, fish, reptiles, mammals, and finally, humans. One must keep in mind the reactivity to subunits such as enzymes, organelles, cells, and membranes. Toxicology has progressed in a few decades from a very necessary, but dreary subject, to a fascinating area where all of the advanced ideas from chemistry, biology, and medicine come together.

A person or an animal might be regarded as an immensely complex swarm of chemical reactions evolving from zygote to embryo, to fetus, to child, and finally to adult. During this evolution, various aspects of the swarm of reactions wax and wane. The swarm changes character constantly as uncounted numbers of chemicals enter the system as food, drugs, drink, and air and influence it. We have by no means characterized all of the elements in the many spices, herbs,

fruits, vegetables, cigarette smoke, engine exhaust, etc. The rather recent discovery of the "food mutagens" that are carcinogenic and that we consume daily came as a complete surprise. They are much more potent than the polycyclic aromatic hydrocarbons long known to occur in burnt food and coal smoke.

Clearly, there are many points of departure in the study of chemical-biological interactions, and one can feel as though one is working at the center of a problem in many different compartments. What we are attempting in this relatively small book is obviously superficial, but this seems to be the only way to make a start.

Our approach will be largely limited to that stemming from physical organic chemistry, and initiated by L. P. Hammett about 1935. That is, the use of experimentally determined parameters from model systems. The basic philosophy is that the structural changes that affect the biological activities of a set of congeners are of three major types: electronic, steric, and hydrophobic. Other factors, such as hydrogen bonding, polarizability, and dipole moment, appear to play less important roles, at least with the tools we now have available. To date, electronic variations have been largely treated using Hammett  $\sigma$  constants or  $pK_a$  values, although molecular-orbital parameters are gaining in importance. Hydrophobic changes are modeled with partition coefficients ( $\log P$  or  $\pi$ ) from the octanol-water system. The most formidable problem of all, that of accounting for the role of geometry or three-dimensional (3-D) shape of the chemicals, has not been addressed in a general way. We cannot do so without a good 3-D model of the receptor's active site. In principle, by studying the perturbations in a cell or mouse from "enough" molecular probes, some salient features of the receptors should be deducible. In a rough analogy, it would be like analyzing the very large number of diffractions from X-rays interacting with a crystal of protein to deduce the protein structure. In the bioreceptor, our problems encounter countless side reactions with other receptors, metabolism, elimination, etc. If specific electronic effects, hydrophobicity, and hydrogen bonding can be more or less accounted for, then the remaining variance can be distributed among steric interactions. Ideally, the problem should be approached on three levels: isolated enzyme, intact cell, and whole animal. As yet, the resources have not been available for anyone to study a well-designed set of, for example, 100 congeners in all three systems.

At present, small steric effects of ordinary substituents can be accounted for rather well, but little information can be obtained about the overall shape of the active site.

We make no attempt to deal with the problem of predicting inactivity as such. Because we cannot find the log of  $O$ , such data cannot be included in a QSAR; however, when the QSAR is obtained, if the inactive compounds are "congeners", the predicted activity should obviously be very low. The problem of predicting inactive compounds in a global sense is not soluble, at least at present. Among the universe of chemicals, the vast majority will be inactive in almost any specific assay, and thus it will be a long time before the multitude of reasons behind inactivity can be sorted out. In the meantime, if one simply guesses that all chemicals will be inactive for a specific type of activity, one will find a good correlation if a large enough set of compounds is considered.

Linear free-energy relationships (LFER) in general and the Hammett equation in particular have been criticized because of their empirical nature and because of their inaccurate results, that is, for lack of perfection. Applying the same high standards for acceptance would undoubtedly cause much, if not all, of science to be rejected. Some medicinal chemists have lost faith in QSAR

when it failed to accurately predict the biological activity of a "near congener". One must bear in mind that all LFERs are bound to fail sooner or later as incremental changes in structure accumulate to differentiate an analog from those upon which the relationship was based. This failure does not mean that "all is lost". The point of failure is a new point of departure to increase one's understanding of the SAR.

Probably no scientific discipline has provided more intellectual satisfaction combined with practical benefit to humankind than has organic chemistry. Yet the successful organic chemist must often rely on a bit of "art" to cover the areas of his science that have yet to be fully explored. The most distinguished of organic chemists have related disastrous experiences when attempting to extend in the laboratory the predictions made in equations contained in textbooks. It is not unusual to take weeks, months, or even years to "work out" the optimum methods for carrying out a multistep synthesis. What teacher of organic chemistry has not carried out a "one-line" reaction in a textbook, found only a 10% yield of the designated product, and only wondered what the other 90% consisted of?

In attacking the problem of inhibiting a receptor inside a pathogenic cell inside an animal, there are no basic laws of chemistry to start with, and one is often in doubt about the numerical values of the biological end point. How pure a number is it? To what extent is it a composite of an interaction with an important receptor and many less important side reactions of all kinds including metabolism? From the beginning, the Pomona school based its approach on time-honored principle of organic chemistry that substituent changes in one series of compounds often parallel those in another series. This approach had been Hammett's guiding principle in formulating his famous equation. He stuck to his position despite objections by the theoretically minded chemists that in correlating free-energy-related processes, he seemed to be ignoring the fact that Gibbs free energy,  $\Delta G$ , depends on both change in enthalpy  $\Delta H$ , and organization energy,  $T\Delta S$ . We still do not completely understand just why the Hammett equation is so generally successful. From the very beginning, the Pomona school had to face the fact that although nonlinear relationships with the Hammett equation are relatively rare, they are very common in biological QSAR; in fact, they are generally expected.

We began with the concept of additivity of the contributions from various physicochemical properties as the first approximation, but progress in QSAR has depended on the use of nonlinear terms, especially hydrophobic and steric. The interaction of the independent variables is an area that has still not been adequately explored. Even as early as 1965, it was all too clear that, in the calculation of  $\log P$  from  $\pi$ , the effect of the electronic interactions of substituents on each other had to be taken into account. This need for study of the independent variables became even more apparent as the CLOGP program for the calculation of partition coefficients from molecular fragments began to evolve. The success of the concept of additivity of fragments to explain the properties of organic molecules, limited as it is, has started many research programs in the area of structure-activity relationships.

The normal test of a QSAR's ability to account for reality is to make and test new congeners with properties both inside and outside of explored data space to assess its predictability. This in-depth validation is important, but it is not the ultimate test of whether or not we are on the right track in a general sense. There are so many published examples for which two or more apparently



different approaches can be used to produce QSAR with more or less the same explanatory power. Lateral validation is, we believe, the only ultimate test. By this statement we mean the establishment of large self-consistent matrices of QSAR not only from widely different biological systems but also including appropriate QSAR from basic organic reactions in simple solvents. To accomplish a paradigm change in the way we do structure-activity analysis is going to be a huge task. Wherever possible in our writing, we have drawn attention to the adage that similar reactions will have similar characteristics (similar terms in the QSAR).

Of course, to do this one needs a common set of parameters. In developing the book, we have tried to limit our examples and discussion to the most generally accepted parameters, realizing that changes are occurring and will continue to occur in just how this should be done.

To make significant progress in the development of a cohesive approach to QSAR requires the ready availability of large numbers of QSAR. One cannot search the literature every time a new idea or area of QSAR is to be analyzed. Only with a computerized database with a smoothly interacting model-building program can we begin seriously to work on the problem of lateral validation. Currently, our program is based on only about 6000 QSAR, but even so, it was invaluable in writing this book.

A crucial factor in advancing QSAR is the best possible database of parameters. In constructing our Tables of Physicochemical Parameters, we tried to be comprehensive rather than critical; that is, we have not attempted to pass judgment on the quality of all of the values, although we do indicate the ones we normally prefer. When there is an obvious discrepancy, we leave it up to the user to consult the original literature to decide whether the model system is appropriate, or whether experimental conditions cast doubt on its validity. Finally, even after considerable cross-checking, we know there must be a number of outright errors in these tables. We would greatly appreciate our readers taking the time to point them out to us.

In conclusion, one cannot expect more success in the rationalization of chemical reactions in the highly heterogeneous milieu of an animal or even a cell than can be achieved with ordinary organic reactions in solution.

### Acknowledgments

We are indebted to Teri Klein of the Molecular Graphics Laboratory at the University of California in San Francisco for composing the stereo pictures in Chapter 7. We would not have been able to make many of the interesting comparisons of QSAR were it not for the help of an excellent computer program written for this purpose by David Hoekman. We are especially thankful to Toshio Fujita for helpful suggestions and for correcting many errors. In addition Mathew Ames, William Denny, Teri Klein, Hugo Kubinyi, C. A. Ramsden, Cynthia Selassie, Peter and Jacqueline Sinclair, Carlo Silipo, Robert Taft, Chiyoza Takayama, and Richard Weinshilboum read and commented on various parts of the manuscript.

We thank Patricia Arms for the many hours of word and formula processing necessary to complete the manuscript.

# **Dedication**

We dedicate this book to our wives, Gloria and Georganna, without whose support this book would not have been possible.

# How To Use the Tables in this Volume

## Octanol LogP

The values in this table are arranged by molformula within the standard categories: carbon, hydrogen, and any other elements in alphabetical order. Reading left to right, the table is arranged as follows:

- The first column gives arbitrary index numbers, which are separated in groups of five to facilitate reading across the row.
- The second column may contain the symbol \*, which designates the preferred value measured as or converted to the neutral form, or the symbol √, which designates a “good” value measured as the ion or a tautomeric mixture.
- The third column contains the log *P* value. If there is more than one value for the same solute, they are in ascending order.
- The fourth contains the pH of measurement.
- The fifth contains the reference number.
- The sixth contains the footnote number. Because the footnote may contain very important information, such as methodology (for example, HPLC) or buffer type, it should always be consulted.
- The seventh column contains the molformula. If the initial molformula ends with a period, it is followed by the formula for the counter ion.
- The eighth column is the solute name. An NSC# (National Cancer Society number) is considered a valid name, as are some commercial laboratory numbers, such as SKF#525. When available, the CAS Registry number follows in boldface type. Because it was not always possible to list the IUPAC name, several shortcuts have been used:
  1. Sometimes common groups are abbreviated, such as NO<sub>2</sub>, and CF<sub>3</sub>, DIAM for diamino, or DIME for dimethyl.
  2. Some peptides are listed by three-letter abbreviations, such as ALA-LEU-PHE, and blocked peptides are listed by AC-ALA-ALA-N.
  3. In a few complex solutes the typewritten structure is given, such as #4977 4-ME-1,2,5-

THIADIAZOLE-3-C(=NOH)SCH<sub>2</sub>CH<sub>2</sub>N(ET)<sub>2</sub>. Often these are depicted at the end of the table.

4. Lacking Greek symbols, the following abbreviations are used: A- for alpha; B- for beta; G- for gamma; W- for omega; D- for delta (unsaturation).
5. Saturation positions are indicated but the level is abbreviated; for example, 2,3,4,5-H<sub>4</sub>, is a tetrahydro analog.

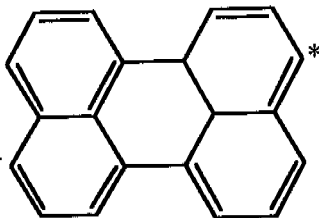
If the name is appended with a heavy cross (+), the structure is depicted in the section at the end of the volume, and the structures are arranged by access number. If depiction is not indicated, and the name leaves some doubt as to the structure, one should look in the immediate vicinity for a similar name that has the structure depicted.

## Hammett Sigmas

This table of electronic, steric, and hydrophobic parameters is based, to a large degree, on the concept of *substituents* on a benzene ring that act upon a particular "probe" moiety (initially Hammett used the ionization of a carboxyl group). This probe is attached to the hydrocarbon ring and is sensitive to differences in the polar character of the substituents under study. Data for a given substituent is accessed via its empirical formula, which is given in the standard order: C<sub>x</sub>H<sub>y</sub> and other elements in alphabetical order. A structural formula is also provided to distinguish substituents with identical empirical formulas. This is given in ordinary typewriter symbols beginning at the attachment bond.

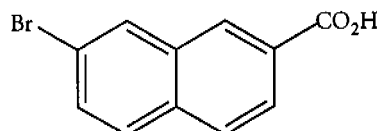
There are two exceptions to the simple *substituent* concept that must be carefully noted and understood:

- 1a. A number of sigma para<sup>+</sup> values have been determined for various positions on polycyclic aromatic rings by pyrolysis or hydrogen exchange of tritiated derivatives (*see* references 699-710). Thus there is neither a "probe" as such nor a "substituent". The position to which the parameter applies is noted by providing a *name* for the entire ring system that takes the place of the structural designation and is followed by a colon. The carbon and hydrogen count for the ring containing the probe is subtracted from the total to get the substituent empirical formula for access. For example, one may want the electronic parameters for the 3-position of perylene

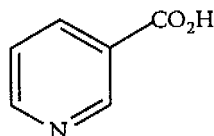


The 3-position establishes which benzene ring is "parent", and the balance of the atom count comes to  $C_{14}H_9$ , which represents the "substituent". The appropriate data is easily found, because the only structural entry besides 3-perylene under this empirical formula is 6-(1,2-benzopyrenyl):

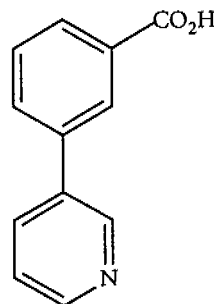
- 1b. When the "active" substituent is on a ring fused to the one with the probe, such as in the bromonaphthoic acid illustrated below, the empirical formula entry is only the benzo-portion,  $C_4H_3BR_1$ , and the structural designation reflects the molecular name [i.e., 2-(7-bromonaphthyl)]:



2. In some heteroaromatic solutes the probe may be on the same ring as the heteroatom that is providing the electronic influence. In this case the electronic parameters may be considered to apply to the heteroatom as a "fused-in" substituent, but the empirical formula used for access will be for the entire ring (minus the probe) and will be followed by the symbol @. A name for the intact ring will be used as the structural formula. It is followed by a colon. Note the difference where the probe is (for example, carboxylic acid ionization):

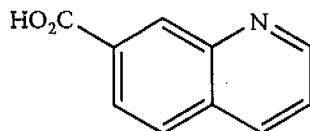


MOLFORMULA =  $C_5H_4N_1@$   
 STRUCT.FORM = 3-pyridyl



$C_5H_4N_1$   
 3-pyridyl

In the "fused-in" case, only sigma meta values appear, while in the "normal" case, all the positional values are possible. When the probe is on a different ring in a fused hetero, such as 7-quinolinyl (shown below), the data is accessed by the substituent empirical formula, e.g.  $C_3H_3N_1@$



If the probe were at the 2-, 3-, or 4-positions, access would be through the empirical formula of the entire molecule:  $C_9H_6N_1@$ .

### Parameter Labels

The left-hand side of each page of the Hammett sigmas table contains those values most frequently used. For more details, see *Exploring QSAR: Fundamentals and Applications in Chemistry and Biology* in the sections noted below:

**$\rho$**  (p) as defined by Fujita and Hansch (4-4-1)

**Sigma meta (S. Meta)** as defined by Hammett (1-1)

**Sigma para (S. Para)** as defined by Hammett (1-1)

**Molar refractivity (M. Refr)** as defined by Hansch et al. (3-5)

**$E_s$  (ES)** as defined by Taft (3-2)

**$E_s^c$**  Taft steric parameter with Hancock's hyperconjugation correction (3-3)

The labels and description of the other parameters listed on the right side of each page are given below. A full discussion for many may be found in *Exploring QSAR: Fundamentals and Applications in Chemistry and Biology* Chapters 1 and 3 or in the appropriate reference in the list at the end of this table.

$\sigma_I$	sigma inductive (51)
$\sigma'$	sigma prime: field effect through bicyclooctane ring (112)
$\sigma_Q$	sigma quinuclidine: field effect on protonated nitrogen (384)
$\sigma^*$	sigma star: aliphatic inductive effect (100; p 587)
$\sigma_m^o$	sigma zero <i>meta</i> : phenylacetic acid ionization or ester hydrolysis (28)
$\sigma_p^+$	sigma plus <i>para</i> : delocalizing +charge; solvolysis of <i>t</i> -cumyl chlorides (15)
$\sigma_m^+$	sigma plus <i>meta</i> (as sigma plus <i>para</i> ) (15)
$\sigma_p^-$	sigma minus <i>para</i> : delocalizing conjugated negative charge; ionization of phenols (P) or anilines (A)
$\sigma_m^-$	sigma minus <i>meta</i> (as sigma minus <i>para</i> )
$\sigma_p^o$	sigma zero <i>para</i> : phenylacetic acid ionization or ester hydrolysis (28)
$\sigma_p^N$	sigma normalized (22)
$\sigma_o$	sigma ortho: various methods (11)
$\sigma_o^+$	sigma plus <i>ortho</i> : delocalizing +charge (355)
$\sigma_o^-$	sigma minus ortho (92)

$\sigma_{\text{R}}^{\text{O}}$	sigma zero resonance: pi-electron delocalization from $\text{C}^{13}\text{NMR}$ (296)
$\sigma_{\text{R}}^{\text{B}}$	sigma benzoic acid resonance: pi-electron delocalization, benzoic acid model (143)
$\sigma_{\text{R}}^{\text{A}}$	sigma aniline resonance: pi-electron delocalization, aniline model (143)
$\sigma_{\text{R}}^{+}$	sigma plus resonance: pi-electron delocalization from <i>t</i> -cumyl chlorides.
ES-A	steric constant: calculated from atomic distances, Austel (667)
ES-CH	steric constant: calculated from atomic distances, Charton (382)
$\text{E}_{\text{s}}^{\text{H}}$	steric constant: hydroboration of substituted ethylenes (252)
$\text{L}_{\text{stm}}$	length of substituent; sterimol calculation (383)
$\text{B}_{1\text{stm}}$	width of substituent; sterimol calculation (383)
$\text{B}_{5\text{stm}}$	width of substituent; sterimol calculation (383)
F	field effect: of Swain & Lupton (modified)
R	resonance effect: of Swain & Lupton (modified)
$\text{R}^{+}$	+resonance effect: resonance delocalization of +charge
$\text{R}^{-}$	-resonance effect: resonance delocalization of -charge
$\sigma_{\text{L}}$	sigma localized: Charton (382)
$\sigma^{\text{F}}$	sigma phosphorus: ionization of phosphorous acids (132)
$\sigma_{\text{Nu}}$	sigma nucleophilic: solvolysis, nucleophilic assistance (491)
$\sigma_{\text{I}}^{\text{F}}$	sigma inductive phosphorus: attached to phosphorus (842)
$\sigma_{\text{R}}^{\text{F}}$	sigma resonance phosphorus: attached to phosphorus (842)
$\sigma_{\text{T}}^{\text{O}}$	sigma zero twist: resonance effect diminished by twisting $90^{\circ}$ out of ring plane (469)
$\sigma_{\text{m}}^{\cdot}$	sigma radical <i>meta</i> : various models (88, 672, 783, 822, 841)
$\sigma_{\text{p}}^{\cdot}$	sigma radical <i>para</i> : various models (88, 672, 783, 822, 841)
$\sigma_{\text{m}}^{\text{c}}$	sigma carbocation <i>meta</i> (678, 754)
$\sigma_{\text{p}}^{\text{c}}$	sigma carbocation <i>para</i> (678, 754)
$\sigma_{\text{Cg}}$	sigma contiguous: delocalization when attached directly to oxygen or nitrogen (645)
$\text{K}_{\text{ap}}$	charge transfer: contribution to electron-donor/acceptor interaction (653)
DP	group dipole: from dipole moment (698)
ELN	group electronegativity (760)
$\sigma^{\Phi+}$	sigma phosphonium: C acidity adjacent to phosphonium
$\text{E}_{\text{s}}^{\text{P}}$	steric pyridinium: quaternerized with MeI

# Octanol LogP





## Octanol LogP

3

	logP	pH	Ref.	Note	MF	Name / CAS / activity
1 ★	0.74		552	400	Ar1	ARGON 7440-37-1
2	-2.95		2358	200	(Cl1)2.Cd1	CADMIUMCHLORIDE
3 ✓	-2.59		2358	200		CADMIUMCHLORIDE
4	-2.47		2019		Cl2Sn1	STANNOUS CHLORIDE 82171-37-3
5	-3.26		2019		Cl4Sn1	STANNIC CHLORIDE 7448-78-8
6 ★	1.68		547	400	F8S1	SULFUR HEXAFLUORIDE 2551-62-4
7 ★	0.28		552	400	He1	HELIUM 7440-59-7
8 ★	-0.22	7.4	2071		Hg1.(Cl1)2	MERCURIC CHLORIDE 7487-94-7
9 ✓	2.49		536		I2	IODINE 7553-58-2 <i>anti-infective (topical)</i>
10 ★	0.89		552	400	Kr1	KRYPTON 7439-90-9
1 ★	0.67		552	400	N2	NITROGEN 7727-37-9
2	0.36		552	500	N2O1	NITROUS OXIDE 10024-97-2
3 ✓	0.43		552	400	N2O1	NITROUS OXIDE
4 ★	0.28		552	400	Ne1	NEON 7440-01-9
15 ★	0.65		552	400	O2	OXYGEN 7782-44-7
6	-3.88	7.4	903	1	Rh1.(Cl1)3	RHODIUM CHLORIDE 10048-07-7
7 ★	1.51		2581		Rn1	RADON 10043-92-2
8	1.15	7.0	1232	1	Xe1	XENON 7440-63-3
9 ★	1.28		552	400		XENON
20 ★	0.45		552	400	H2	HYDROGEN 1333-74-0
1	-1.06		1237		H2O1	TRITIUM OXIDE 13670-17-2
2 ★	-1.38		500		H2O1	WATER 7732-18-6
3	-1.15	7.4	2306	1	"	WATER
4	-3.40	7.4	1237	1	H2O4P1.Na1	SODIUM ION (PHOSPHATE BUFFER)
25	-1.86		1670		H3O4P1	PHOSPHORIC ACID 7664-38-2
6 ✓	-2.07		579		H4N2	HYDRAZINE 302-01-2
7 ✓	-2.19		2426	537	H6C12N2P11	CISPLATIN 15663-27-1 <i>antineoplastic</i>
8	-1.43		564		"	CISPLATIN
9 ✓	-1.43		564	452	H6C12N2P11	DIAMINE-DICHLOROPLATINUM-CIS
30 ✓	-3.36		2426		H10N2O2P11.(N1O3)2	PLATINUM,DIAMMONIO-DIAQUA-DINITRATE
1 ★	1.86		547	400	C1Br1F3	BROMOTRIFLUOROMETHANE 75-63-8
2 ★	2.67		594		C1Br3	BROMOFORM 75-25-2 <i>sedative, antitussive</i>
3 ★	3.42		594	400	C1Br4	CARBON TETRABROMIDE 558-13-4
4 ★	1.08		547	400	C1Cl1F2	CHLORODIFLUOROMETHANE 75-45-6
35 ★	1.65		547	400	C1Cl1F3	CHLOROTRIFLUOROMETHANE 75-72-9
6 ★	1.55		547	400	C1Cl2F1	DICHLOROFLUOROMETHANE 75-43-4
7 ★	2.16		547	400	C1Cl2F2	DICHLORODIFLUOROMETHANE 75-71-8
8 ★	1.97		503		C1Cl3	CHLOROFORM 67-68-3 <i>solvent, anesthetic (vet)</i>
9	1.95		547	160	C1Cl3	DEUTEROCHLOROFORM 1111-69-3
40 ★	2.53		547	400	C1Cl3F1	TRICHLOROFLUOROMETHANE 75-69-4
1 ★	2.09		579		C1Cl3N1O2	CHLOROPICRIN 78-06-2
2 ★	2.83		547	400	C1Cl4	CARBON TETRACHLORIDE 56-23-5 <i>solvent, anthelmintic</i>
3 ★	0.64		547	400	C1F3	FLUOROFORM 75-46-7
4 ★	1.18		552	400	C1F4	TETRAFLUOROMETHANE 75-73-0
45 ★	-0.25		547	400	C1N1	HYDROCYANIC ACID 74-90-8
6	0.32		1262		C1N1S1	HYPOTHIOCYANOUS ACID
7 ★	0.83		2466	716	C1O2	CARBONDIOXIDE 124-38-9
8	-2.81		536		C1S1.Na1	SODIUMTHIOCYANATE 540-72-7
9 ★	1.94		579		C1S2	CARBON DISULFIDE 75-15-0
50 ★	1.41		1560	100	C1H2Br1Cl1	BROMOCHLOROMETHANE 74-97-5
1 ★	1.88		594		C1H2Br2	DIBROMOMETHANE 74-95-3
2 ★	1.25		547	400	C1H2Cl2	METHYLENECHLORIDE 75-09-2
3 ★	0.20		547	400	C1H2F2	DIFLUOROMETHANE 75-10-5
4 ★	2.30		592		C1H2I2	DIODOMETHANE 75-11-6
55 ★	-0.60		924		C1H2N4	TETRAZOLE 288-84-6
6 ★	0.35		1322		C1H2O1	FORMALDEHYDE 50-00-0
7 ★	-0.54		510		C1H2O2	FORMIC ACID 64-18-6
8 ★	1.19		547	400	C1H3Br1	METHYLBROMIDE 74-83-9
9 ★	0.91		547	400	C1H3Cl1	METHYLCHLORIDE 74-87-3 <i>anesthetic (local), refrigerant</i>
60 ★	0.41	7.4	2071		C1H3Cl1Hg1	METHYL MERCURIC CHLORIDE 115-09-3 <i>fungicide</i>
1 ★	0.51		547	400	C1H3F1	METHYLFLUORIDE 593-53-3
2 ★	0.55	1.0	590		C1H3F1O2S1	METHANESULFONYL FLUORIDE 558-25-8
3 ★	1.51		547	400	C1H3I1	METHYL IODIDE 74-88-4
4 ★	-1.51		572		C1H3N1O1	FORMAMIDE 75-12-7
65 ★	-0.35		547	400	C1H3N1O2	NITROMETHANE 75-52-5
6 ★	1.09		547	400	C1H4	METHANE 74-82-8
7 ★	-2.05		1137		C1H4N2O1	FORMIC ACID HYDRAZIDE 624-84-0
8 ★	-2.11		547		C1H4N2O1	UREA 57-13-6 <i>diuretic</i>
9	-1.66	7.4	1237	1	"	UREA
70 ★	-1.80		401		C1H4N2O2	HYDROXYUREA 127-07-1 <i>antineoplastic</i>
1	-1.27	7.4	1184	1	"	HYDROXYUREA
2 ★	-1.02		1087		C1H4N2S1	THIOUREA 62-56-6
3	-0.89		1173	537	C1H4N4O2	2-NITROGUANIDINE 566-88-7
4 ★	-0.77		547	60	C1H4O1	METHANOL 67-56-1 <i>pharmaceutical aid (solvent)</i>
75	-0.50	7.4	2306	1	"	METHANOL
6	-0.32	7.4	1758	1	"	METHANOL
7	-3.10		1189		C1H5As1O3	MONOSODIUM METHANEARSONATE 2163-80-6
8 ★	-0.57		510		C1H5N1	METHYLAMINE 74-89-5
9 ★	-2.75		1394		C1H5N3O1	SEMICARBAZIDE 563-41-7
80 ★	-1.05	13.0	579	224	C1H8N2	METHYLHYDRAZINE 60-34-4
1 ★	2.82		547	400	C2Cl2F4	1,2-DICHLOROTETRAFLUOROETHANE 76-14-2
2 ★	3.16		1369	459	C2Cl3F3	1,1,2-TRICHLOROTRIFLUOROETHANE 76-13-1
3 ★	2.09		579		C2Cl3N1	TRICHLOROACETONITRILE 545-06-2 <i>insecticide</i>
4 ★	3.40		579		C2Cl4	TETRACHLOROETHYLENE 127-18-4 <i>anthelmintic</i>
85 ★	4.14		2000		C2Cl6	HEXACHLOROETHANE 67-72-1
6 ★	2.00		552	400	C2F6	HEXAFLUOROETHANE 76-18-4
7 ★	0.07		579		C2N2	CYANOGEN 480-19-5
8	1.70	7.0	1232	1	C2H1Br1Cl1F3	HALOTHANE 151-67-7 <i>anesthetic (inhalation)</i>
9 ★	2.30		547	60	"	HALOTHANE

## Exploring QSAR: Hydrophobic, Electronic, and Steric Constants

	logP	pH	Ref.	Note	MF	Name / CAS / activity
90	★	2.24	509		C2H1Br2N3	1,2,4-TRIAZOLE,3,5-DIBROMO 7411-23-6
1	★	3.20	1683		C2H1Br3	TRIBROMOETHENE 599-16-3
2	★	2.61	2605		C2H1Cl3	TRICHLOROETHYLENE 79-01-6 <i>analgesic (inhalation), anesthetic (inhalant, vet)</i>
3	★	1.33	572		C2H1Cl3O2	TRICHLOROACETIC ACID 76-03-9 <i>caustic</i>
4	★	3.22	579		C2H1Cl5	PENTACHLOROETHANE 76-01-7
95	★	0.37	547	400	C2H2	ACETYLENE 74-86-2
6	★	0.45	579		C2H2Cl1N1	CHLOROACETONITRILE 107-14-2
7	★	2.13	572		C2H2Cl2	1,1-DICHLOROETHYLENE 75-35-4
8	★	1.86	572		C2H2Cl2	CIS-1,2-DICHLOROETHYLENE 156-59-2
9	★	2.09	572		C2H2Cl2	TRANS-1,2-DICHLOROETHYLENE 156-60-5
100	★	0.92	572		C2H2Cl2O2	DICHLOROACETIC ACID 79-43-6
1	★	1.04	508		C2H2Cl3N1O1	TRICHLOROACETAMIDE 594-65-0
2	★	2.39	1179		C2H2Cl4	1,1,2,2-TETRACHLOROETHANE 79-34-5
3	★	1.24	547	400	C2H2F2	1,1-DIFLUOROETHYLENE 75-38-7
4	★	0.12	528		C2H2F3N1O1	TRIFLUOROACETAMIDE 354-38-1
5	★	0.16	2166		C2H2N2O1	FURAZAN 298-37-8
6	★	-0.33	2592		C2H2N4O2	1H-1,2,4-TRIAZOLE,3-NITRO
7	★	1.57	572		C2H3Br1	VINYLBROMIDE 593-60-2
8	★	0.41	510		C2H3Br1O2	BROMOACETIC ACID 79-08-3
9	★	2.10	591		C2H3Br3O1	TRIBROMOETHANOL 75-80-9 <i>anesthetic (inhalation)</i>
110	★	2.79	579		C2H3Cl1	CHLOROETHYLENE 75-01-4
1	★	0.22	572		C2H3Cl1O2	CHLOROACETIC ACID 79-11-8
2	★	0.19	594		C2H3Cl2N1O1	ACETAMIDE,2,2-DICHLORO 683-72-7
3	★	2.49	547	400	C2H3Cl3	1,1,1-TRICHLOROETHANE 71-55-6
4	★	1.89	590		C2H3Cl3	1,1,2-TRICHLOROETHANE 79-00-5
15	★	1.42	7.4	404	1 C2H3Cl3O1	2,2,2-TRICHLOROETHANOL 115-20-8
6	★	0.99	579		C2H3Cl3O2	2,2,2-TRICHLORO-1,1-ETHANEDIOL 302-17-0 <i>hypnotic, sedative</i>
7	★	1.61	7.4	404	1	2,2,2-TRICHLORO-1,1-ETHANEDIOL
8	★	0.41	506		C2H3F3O1	2,2,2-TRIFLUOROETHANOL 75-89-8
9	★	-0.34	503		C2H3N1	ACETONITRILE 75-05-8
120	★	0.94	1947		C2H3N1S1	METHYLISOTHIOCYANATE 556-61-6 <i>pesticide</i>
1	★	-0.58	590		C2H3N3	1H-1,2,4-TRIAZOLE 288-86-0
2	★	-0.29	924		C2H3N3	2H-1,2,3-TRIAZOLE 286-36-8
3	★	-1.44	1137		C2H3N3O1	2-AMINO-1,3,4-OXADIAZOLE 3775-60-8
4	★	-0.57	7.4	401	1 C2H3N3S1	2-AMINO-1,3,4-THIADIAZOLE 4005-51-0 <i>antineoplastic</i>
25	✓	-1.18	7.4	903	1 (C2H3O2)4.(Rh1)2	RHODIUM(II)ACETATE
6	★	1.13	547		C2H4	ETHYLENE 74-85-1
7	★	-0.52	528		C2H4Br1N1O1	BROMOACETAMIDE 683-57-8
8	★	1.96	579		C2H4Br2	1,2-DIBROMOETHANE 106-93-4
9	★	-0.53	508		C2H4Cl1N1O1	CHLOROACETAMIDE 79-07-2
130	★	1.10	594		C2H4Cl1N1O2	ETHANE,1-CHLORO-1-NITRO 596-92-5
1	★	1.79	547	400	C2H4Cl2	1,1-DICHLOROETHANE 75-34-3
2	★	1.48	547	400	C2H4Cl2	1,2-DICHLOROETHANE 107-06-2
3	★	0.37	425		C2H4Cl2O1	2,2-DICHLOROETHANOL 598-38-9
4	★	-1.05	528		C2H4F1O1	FLUOROACETAMIDE 840-19-7
35	★	0.75	547	400	C2H4F2	1,1-DIFLUOROETHANE 75-37-6
6	★	0.24	1701		C2H4F3N1	ETHYLAMINE,2,2,2-TRIFLUORO 753-90-2
7	★	-0.19	528		C2H4I1O1	IODOACETAMIDE 144-48-9
8	★	2.71	7.4	579	1 C2H4I2	1,2-DIODOETHANE 824-73-7
9	★	-1.37	13.0	579	C2H4N2	ACETONITRILE,AMINO 540-61-4
140	★	1.16	1358		C2H4N2O6	ETHYLENEGLYCOLDINITRATE 628-96-6
1	★	-1.15	1173	537	C2H4N4	2-CYANOGLUANIDINE 481-58-5
2	★	-0.87	2660		C2H4N4	AMITROLE 61-82-5 <i>herbicide</i>
3	★	-0.84	2667	226	"	AMITROLE
4	★	-0.49	2166		C2H4N4O1	1,2,5-OXADIAZOLE,3,4-DIAMINO
45	★	-0.90	5.4	284	C2H4N4O2S2	2-AMINO-1,3,4-THIADIAZOLE-5-SULFONAMIDE
6	★	-0.30	547	400	C2H4O1	ETHYLENEOXIDE 75-21-8
7	★	-0.17	505		C2H4O2	ACETIC ACID 64-19-7
8	★	0.03	599		C2H4O2	METHYLFORMATE 107-31-3
9	★	0.09	547		C2H4O2S1	MERCAPTOACETIC ACID 68-11-1
150	★	-1.11	510		C2H4O3	HYDROXYACETIC ACID 79-14-1
1	★	1.61	547	400	C2H5Br1	ETHYLBROMIDE 74-96-4
2	★	0.18	594		C2H5Br1O1	2-BROMOETHANOL 540-51-2
3	★	1.43	547	400	C2H5Cl1	ETHYLCHLORIDE 75-00-3 <i>anesthetic (topical)</i>
4	★	-0.06	594		C2H5Cl1O1	2-CHLOROETHANOL 107-07-3
55	★	-0.20	2019		C2H5Cl3Sn1	TRICHLOROSTANNANE,ETHYL 1066-57-5
6	★	-0.78	594	400	C2H5F1O1	2-FLUOROETHANOL 371-82-0
7	★	2.00	503		C2H5I1	ETHYL IODIDE 75-03-6
8	★	-0.13	508		C2H5N1O1	ACETALDOXIME 107-29-8
9	★	-1.26	1087		C2H5N1O1	ACETAMIDE 60-35-5
160	★	-0.97	594	400	C2H5N1O1	METHYLFORMAMIDE 123-39-7 <i>antineoplastic</i>
1	★	-1.59	579		C2H5N1O2	ACETOHYDROXAMIC ACID 546-88-3 <i>enzyme inhibitor (urease)</i>
2	★	-3.21	547	463	C2H5N1O2	GLYCINE 58-06-8 <i>nutrient</i>
3	★	0.18	547	400	C2H5N1O2	NITROETHANE 79-24-3
4	★	-0.66	7.4	172	1 C2H5N1O2	O-METHYLCARBAMATE 598-55-0
65	★	-0.42	547		C2H5N1O3	2-NITROETHANOL 625-48-9
6	★	-0.26	579		C2H5N1S1	THIOACETAMIDE 62-55-5
7	★	-0.03	401		C2H5N3O2	1-METHYL-1-NITROSOUREA 684-93-5
8	★	-1.61	401	1	C2H5N5	GUANAZOLE 1455-77-2 <i>antineoplastic</i>
9	★	-1.61	7.4	401	1	GUANAZOLE
170	★	1.81	547	400	C2H6	ETHANE 74-84-0
1	★	-0.96	7.0	2625	1 C2H6Cl1O3P1	ETHEPHON 11672-87-0 <i>growth regulator</i>
2	★	-3.03	2019		C2H6Cl2Sn1	DICHLOROSTANNANE,DIMETHYL 753-73-1
3	★	2.59	547		C2H6Hg1	DIMETHYLMERCURY 593-74-8
4	★	-1.58	1137		C2H6N2O1	ACETIC ACID HYDRAZIDE 1068-57-1

logP	pH	Ref.	Note	MF	Name / CAS / activity
75 ★	-1.40	2198		C2H6N2O1	METHYLUREA 598-50-5
6 ★	-0.57	871		C2H6N2O1	N-NITROSODIMETHYLAMINE 62-75-9
7 ★	-0.46	7.4 1184	1	C2H6N2O2	1-METHYL-1-HYDROXYUREA 7433-43-4
8 ★	-0.68	1173	537	C2H6N2S1	METHYLTHIOUREA 598-62-7
9 ★	0.10	547	400	C2H6O1	DIMETHYLETHER 115-10-6
180 ★	-0.37	7.0 1232		1 C2H6O1	ETHANOL 64-17-5 solvent, anti-infective
1 ★	-0.31	547	400	"	ETHANOL
2	-0.22	7.2 2016		"	ETHANOL
3 ★	-1.35	540		C2H8O1S1	DIMETHYLSULFOXIDE 67-68-5 anti-inflammatory (topical)
4 ★	-1.36	572		C2H6O2	ETHANE-1,2-DIOL 107-21-1
85 ★	-1.34	594	400	C2H6O2S1	METHYLSULFONE 67-71-0
6 ★	1.77	536		C2H6S2	DIMETHYL DISULFIDE 624-92-0
7 ★	-0.38	13.0 1013	821	C2H7N1	DIMETHYLAMINE 124-40-3
8 ★	-0.13	13.0 588	224	C2H7N1	ETHYLAMINE 75-04-7
9 ★	-1.31	510		C2H7N1O1	ETHANOLAMINE 141-43-5 sclerosing agent
190 ★	-1.15	13.0 594		C2H7N1O1	METHANAMINE, N-HYDROXY, N-METHYL 5725-96-2
1 ★	-2.20	1394		C2H7N3O1	4-METHYLSEMICARBAZIDE 17696-95-6
2	-0.66	600		C2H8N1O2P1S1	METHAMIDOPHOS 10265-92-6 insecticide
3 ★	-2.04	13.0 579		C2H8N2	ETHYLENE DIAMINE 107-15-3 urinary acidifier (vet)
4 ✓	-1.68	2426	537	C2H10Cl2N2P1	PLATINUM, BIS-METHYLAMMONIO-DICHLORO
95 ✓	-3.28	2426		C2H14N2O2P11, (N1O3)2	PLATINUM, BIS-METHYLAMMONIO-DIAQUA-DINITRATE
6 ★	1.46	579		C3F6O1	HEXAFLUOROACETONE 10057-27-9
7 ★	2.82	2137		C3H1Br2N3O2	IMIDAZOLE, 2,4-DIBROMO-5-NITRO
8 ★	1.96	509		C3H1Br3N2	IMIDAZOLE, 2,4,5-TRIBROMO 2034-22-2
9 ★	1.85	509		C3H1Cl3N2	IMIDAZOLE, 2,4,5-TRICHLORO 7682-38-4
200 ★	2.78	509		C3H1I3N2	IMIDAZOLE, 2,4,5-TRIIODO 1746-25-4
1 ★	0.71	2387		C3H2Br1N3O2	IMIDAZOLE, 2-BROMO-4-NITRO 65902-59-2
2 ★	0.85	2387		C3H2Br1N3O2	IMIDAZOLE, 4-NITRO-5-BROMO 6963-65-1
3 ★	2.10	547	400	C3H2Cl1F5O1	2-CL-1,1,2-TRIFLUORO-2,2,2-TRIFLUOROETHANE 13838-16-9 anesthetic (inhalation)
4 ★	2.06	591		C3H2Cl1F5O1	ISOFLURANE 26675-48-7 anesthetic (inhalation)
5 ★	0.66	2387		C3H2Cl1N3O2	IMIDAZOLE, 2-CHLORO-4-NITRO 57531-37-0
6 ★	0.78	2387		C3H2Cl1N3O2	IMIDAZOLE, 4-NITRO-5-CHLORO 57531-38-1
7 ★	1.66	590		C3H2F6O1	HEXAFLUORO-2-PROPANOL 920-66-1
8	0.28	7.4 1975	1	C3H2I1N3O2	IMIDAZOLE, 4-NITRO-5-IODO 76529-48-1
9 ★	-0.50	579		C3H2N2	MALONONITRILE 109-77-3
210 ★	0.20	2387		C3H2N4O4	IMIDAZOLE, 2,4-DINITRO 5213-49-0
1 ★	0.85	2387		C3H2N4O4	IMIDAZOLE, 4,5-DINITRO 18183-14-3
2 ★	1.02	2166		C3H3Cl1N2O2	FURAZAN-2-OXIDE, 3-METHYL-4-CHLORO
3 ★	0.90	2166		C3H3Cl1N2O2	FURAZAN-2-OXIDE, 4-METHYL-3-CHLORO
4 ★	2.03	594		C3H3Cl3O2	TRICHLOROACETIC ACID, METHYL ESTER 598-99-2
15	0.20	579		C3H3F3O1	1,1,1-TRIFLUOROACETONE 421-50-1
6 ★	0.60	594	400	C3H3F3O2	TRIFLUOROACETIC ACID, METHYL ESTER 431-47-0
7 ★	1.23	506		C3H3F5O1	PROFANOL, 2,2,3,3,3-PENTAFLUORO 422-05-9
8 ★	1.70	547		C3H3I1N2	4-IODOPYRAZOLE 3469-69-0
9 ★	0.25	570	400	C3H3N1	ACRYLONITRILE 107-13-1
220 ★	0.08	508		C3H3N1O1	ISOXAZOLE 288-14-2
1 ★	0.12	1627		C3H3N1O1	OXAZOLE 288-42-6
2 ★	-0.76	1.0 594	342	C3H3N1O2	CYANOACETIC ACID 372-09-8
3 ★	0.44	505		C3H3N1S1	THIAZOLE 288-47-1
4	-0.73	7.4 1163	1	C3H3N3	SYM-TRIAZINE 290-87-9
25	0.66	7.4 1094	1	C3H3N3O1S1	1,2,3-THIAZOLE-5-CARBOXALDOXIME 61444-94-8
6 ★	0.86	7.4 1094	2	"	1,2,3-THIAZOLE-5-CARBOXALDOXIME
7	-0.34	7.4 2206	306	C3H3N3O2	2-NITROIMIDAZOLE 527-73-1
8 ★	0.15	1008	354	"	2-NITROIMIDAZOLE
9 ★	-0.11	1008	354	C3H3N3O2	4-NITROIMIDAZOLE 3034-38-6
230 ★	0.59	547		C3H3N3O2	4-NITROPYRAZOLE 2075-46-9
1 ★	-1.87	924	400	C3H3N3O2	5-AZACITRIL 71-33-0
2	-0.17	7.4 2206	306	C3H3N3O2	5-NITROIMIDAZOLE 3034-38-6
3 ★	-0.01	9.0 1409	2	"	5-NITROIMIDAZOLE
4	-1.37	7.4 579	1	C3H3N3O2	6-AZACITRIL 461-89-2
35 ★	-0.59	7.4 579	2	"	6-AZACITRIL
6 ★	0.83	594		C3H3N3O2S1	THIAZOLE, 2-AMINO-5-NITRO 121-66-4 antihistomonad in fowl
7 ★	0.97	2166		C3H3N3O3	1,2,5-OXADIAZOLE, 3-NITRO-4-METHYL
8 ★	0.78	2166		C3H3N3O4	FURAZAN-2-OXIDE, 3-METHYL-4-NITRO
9 ★	1.45	547	400	C3H4	ALLENE 463-48-0
240 ★	0.94	547	400	C3H4	METHYLACETYLENE 74-99-7
1 ★	0.18	1896		C3H4Cl1N1	3-CHLOROPROPIONITRILE 1617-17-0
2 ★	2.21	530		C3H4Cl2F2O1	METHOXYFLURANE 76-38-0 anesthetic (inhalation)
3	0.78	1178		C3H4Cl2O2	DALAPON 75-99-0 herbicide
4 ★	-0.08	259		C3H4N2	IMIDAZOLE 288-32-4
45 ★	0.26	547		C3H4N2	PYRAZOLE 286-13-1
6 ★	-0.18	1625		C3H4N2O1	OXAZOLE-2-AMINE 4570-45-0
7 ★	-1.69	508		C3H4N2O2	HYDANTOIN 461-72-3
8 ★	0.38	572		C3H4N2S1	2-AMINOTHIAZOLE 96-50-4 thyroid inhibitor
9 ★	-0.68	7.4 2273	1	C3H4N4O2	1,2,4-TRIAZOLE, 1-METHYL-3-NITRO 26621-45-4
250 ★	-0.38	579		C3H4O1	PROPARGYL ALCOHOL 107-19-7
1 ★	-0.01	572		C3H4O1	PROPENAL 107-02-8 herbicide
2 ★	0.35	1.0 594		C3H4O2	ACRYLIC ACID 79-10-7
3 ★	-0.81	1.0 594	342	C3H4O4	MALONIC ACID 141-82-2
4 ★	1.79	1560	459	C3H5Br1	ALLYLBROMIDE 106-95-6
55 ★	0.85	2219		C3H5Br1O1	EPIBROMOHYDRIN 3132-64-7
8 ★	0.92	510		C3H5Br1O2	A-BROMOPROPIONIC ACID 598-72-1
7 ★	2.00	579	400	C3H5Cl1	PROPENE, 2-CHLORO 657-98-2
8 ★	0.45	2219		C3H5Cl1O1	EPICHLOROHYDRIN 106-89-8
9 ★	0.41	1.0 594	400	C3H5Cl1O2	B-CHLOROPROPIONIC ACID 107-94-8

## Exploring QSAR: Hydrophobic, Electronic, and Steric Constants

logP	pH	Ref.	Note	MF	Name / CAS / activity
260 ★	-0.16	594	400	C3H5F1O1	EPIFLUOROHYDRIN 503-09-3
1 ★	-0.39	579		C3H5F1O1	FLUOROACETONE 430-51-3
2 ★	0.71	425		C3H5F3O1	1,1,1-TRIFLUORO-2-PROPANOL 374-01-6
3 ★	0.39	1942		C3H5F3O1	3,3,3-TRIFLUOROPROPANOL
4 ★	-0.43	594		C3H5N1	2-PROPYN-1-AMINE 2450-71-7
65 ★	0.16	503		C3H5N1	PROPIONITRILE 107-12-0
6 ★	-0.94	1896		C3H5N1O1	3-HYDROXYPROPIONITRILE 78-97-7
7 ★	-0.87	572		C3H5N1O1	ACRYLAMIDE 79-06-1
8 ★	0.34	1094	1	C3H5N1O2	HYDROXYIMINOACETONE 306-44-5
9 ★	0.34	2334			HYDROXYIMINOACETONE
270 ★	0.39	1094	2		HYDROXYIMINOACETONE
1 ★	-1.42	594	400	C3H5N1O2S1	METHYLSULFONYLACETONITRILE 2274-42-2
2 ★	1.47	850		C3H5N1S1	ETHYLISOTHIOCYANATE 542-85-8
3 ★	-0.55	2619		C3H5N3	1,2,4-TRIAZOLE,3-METHYL
4 ★	-1.09	547	224	C3H5N3	4-AMINOPYRAZOLE 28466-26-4
75 ★	-1.64	594	299	C3H5N3	IMIDAZOLE,2-AMINO 1450-83-7
6 ★	0.09	2166		C3H5N3O1	1,2,5-OXADIAZOLE,3-AMINO-4-METHYL
7 ★	-0.92	1137		C3H5N3O1	2-AMINO-5-METHYL-1,3,4-OXADIAZOLE 52838-39-8
8 ★	-0.17	2166		C3H5N3O2	FURAZAN-2-OXIDE,3-METHYL-4-AMINO
9 ★	-0.32	2166		C3H5N3O2	FURAZAN-2-OXIDE,4-METHYL-3-AMINO
280 ★	1.62	1358		C3H5N3O9	GLYCERYLTRINITRATE 55-63-0
1 ★	1.72	547	400	C3H6	CYCLOPROPANE 75-19-4 <i>anesthetic (inhalation)</i>
2 ★	1.77	547	400	C3H6	PROPYLENE 115-07-1
3 ★	2.18	1560	100	C3H6Br1Cl1	1-BROMO-3-CHLOROPROPANE 109-70-8
4 ★	2.37	594		C3H6Br2	1,3-DIBROMOPROPANE 109-64-8
85 ★	0.57	401		C3H6Cl1N3O2	1-(2-CHLOROETHYL)-1-NITROSOUREA(NCS47547) 2385-30-2
6 ★	2.00	547		C3H6Cl2	1,3-DICHLOROPROPANE 142-28-9
7 ★	-0.83	594		C3H6F1O1	A-FLUORO-N-METHYLACETAMIDE 367-49-7
8 ★	-0.36	579		C3H6F2O1	1,3-DIFLUORO-2-PROPANOL 453-13-4
9 ★	0.55	1701		C3H6F3N1	N-METHYL-2,2,2-TRIFLUOROETHYLAMINE
290 ★	3.02	579		C3H6I2	1,3-DIIODOPROPANE 627-31-6
1 ★	-0.15	579		C3H6N2	DIMETHYLCYANAMIDE 1467-79-4
2 ★	-0.68	507		C3H6N2S1	IMIDAZOLIDONE,2-THIO 96-45-7
3 ★	-0.77	1173	537	C3H6N4	1-METHYL-2-CYANOQUANIDINE 1609-07-0
4 ★	-1.37	599		C3H6N6	1,3,5-TRIAZINE,2,4,6-TRIAMINO 108-78-1
95 ★	0.87	1179		C3H6N6O6	1,3,5-TRIAZA-1,3,5-TRINITROCYCLOHEXANE 121-82-4 <i>rodenticide, explosive</i>
6 ★	-0.24	510		C3H6O1	ACETONE 67-64-1
7 ★	0.17	508		C3H6O1	ALLYL ALCOHOL 107-18-6
8 ★	0.59	572		C3H6O1	PROPIONALDEHYDE 123-38-6
9 ★	0.03	572		C3H6O1	PROPYLENEOXIDE 75-56-9
300 ★	-0.14	594	400	C3H6O1	TRIMETHYLENE OXIDE 503-30-0
1 ★	-0.37	572		C3H6O2	1,3-DIOXOLANE 646-06-0
2 ★	0.18	510		C3H6O2	ACETIC ACID,METHYL ESTER 79-20-9
3 ★	-0.95	2219		C3H6O2	GLYCIDOL 558-52-5
4 ★	0.33	505		C3H6O2	PROPIONIC ACID 79-09-4 <i>antimicrobial</i>
5 ★	0.43	547		C3H6O2S1	3-MERCAPTPTOPROPIONIC ACID 107-86-0
6 ★	-0.72	986		C3H6O3	A-HYDROXYPROPIONIC ACID 598-82-3
7 ★	-0.43	579		C3H6O3	TRIOXANE 110-88-3
8 ★	2.10	503		C3H7Br1	1-BROMOPROPANE 106-94-5
9 ★	2.14	594	400	C3H7Br1	2-PROMOPROPANE 75-26-3
310 ★	0.02	2071		C3H7Br1Hg1O1	1-BROMOMERCURY-2-HYDROXYPROPANE 18832-83-2
1 ★	2.04	547	400	C3H7Cl1	1-CHLOROPROPANE 540-54-5
2 ★	1.90	547	400	C3H7Cl1	2-CHLOROPROPANE 75-29-6
3 ★	0.50	594	400	C3H7Cl1O1	3-CHLORO-1-PROPANOL 627-30-5
4 ★	-0.28	594	400	C3H7F1O1	PROPANOL,3-FLUORO 462-43-1
15 ★	2.89	594	400	C3H7I1	2-IODOPROPANE 75-30-9
6 ★	0.07	588	224	C3H7N1	ALLYLAMINE 107-11-9
7 ★	0.07	579		C3H7N1	CYCLOPROPYLAMINE 785-30-0
8 ★	0.12	579		C3H7N1O1	ACETONEOXIME 127-08-0
9 ★	-1.01	541		C3H7N1O1	DIMETHYLFORMAMIDE 68-12-2
320 ★	-1.05	536		C3H7N1O1	N-METHYLACETAMIDE 79-16-3
1 ★	-0.66	2226		C3H7N1O1	PROPIONAMIDE 79-05-0
2 ★	0.87	547	60	C3H7N1O2	1-NITROPROPANE 108-03-2
3 ★	0.80	2571		C3H7N1O2	2-NITROPROPANE 79-46-9
4 ★	-3.05	2854	448	C3H7N1O2	3-AMINOPROPIONIC ACID 28854-76-4
25 ★	-2.98	547	463	C3H7N1O2	ALANINE 302-72-7
6 ★	-2.74	1207	1		ALANINE
7 ★	-0.06	702		C3H7N1O2	O,N-DIMETHYLCARBAMATE 6642-30-4
8 ★	-0.15	172	1	C3H7N1O2	O-ETHYLCARBAMATE 51-79-6 <i>antineoplastic</i>
9 ★	-0.15	505			O-ETHYLCARBAMATE
330 ★	0.04	1232	1		O-ETHYLCARBAMATE
1 ★	-2.78	2654	448	C3H7N1O2	SARCOSINE 107-97-1
2 ★	-2.49	1590	459	C3H7N1O2S1	CYSTEINE 52-90-4 <i>amino acid</i>
3 ★	4.32	1323	820	C3H7N1O3	SERINE,TETRAHEXYL AMMONIUM SALT
4 ★	-3.07	1207	1	C3H7N1O3	SERINE 56-45-1 <i>amino acid</i>
35 ★	0.23	8.9	1498	C3H7N3O2	1-ETHYL-1-NITROSOUREA 759-73-9
6 ★	2.36	547	400	C3H8	PROPANE 74-98-6
7 ★	-1.70	1365		C3H8N1O5P1	N-(PHOSPHONOMETHYL)GLYCINE 1071-83-6 <i>herbicide</i>
8 ★	-0.49	547		C3H8N2O1	DIMETHYLUREA,SYM. 96-31-1
9 ★	-0.74	547		C3H8N2O1	ETHYLUREA 625-52-5
340 ★	-0.02	2570		C3H8N2O1	METHYLETHYLNITROSAMINE 10595-95-6
1 ★	-1.00	1137		C3H8N2O1	PROPIONIC ACID HYDRAZIDE 24535-11-3
2 ★	-0.10	1184	1	C3H8N2O2	1-ETHYL-1-HYDROXYUREA 7433-42-3
3 ★	-0.76	1184	1	C3H8N2O2	3-ETHYLHYDROXYUREA 8710-11-2
4 ★	-0.24	1173	537	C3H8N2S1	1,3-DIMETHYLTHIOUREA 534-13-4

logP	pH	Ref.	Note	MF	Name / CAS / activity
45 ★	-0.21	6.5	2013	C3H8N2S1	ETHYLTHIOUREA 625-53-8
6 ★	-0.70	1173	537	C3H8N4O2	1,3-DIMETHYL-2-NITROGUANIDINE
7 ★	0.05	425		C3H8O1	ISOPROPYL ALCOHOL 67-63-0 <i>anti-infective (topical)</i>
8 ★	0.25	547	80	C3H8O1	PROPANOL 71-23-8
9 ★	-0.92	1397	122	C3H8O2	1,2-PROPANEDIOL 57-55-6 <i>pharmaceutical aid (humectant)</i>
350 ★	-1.04	579		C3H8O2	1,3-PROPANEDIOL 504-83-2
1 ★	0.18	579	400	C3H8O2	DIMETHOXYMETHANE 109-87-5
2 ★	-0.77	768		C3H8O2	METHOXYETHANOL 109-86-4
3	-1.79	7.4	1758	1 C3H8O3	GLYCEROL 56-81-5 <i>antiglaucoma</i>
4 ★	-1.76	7.4	1010	1	GLYCEROL
55 ★	1.54	594	400	C3H8S1	ETHYLMETHYL SULFIDE 624-89-5
6 ★	1.81	579		C3H8S1	PROPANETHIOL 107-03-0
7	-0.29	1959		C3H9Cl1Sn1	CHLOROSTANNANE, TRIMETHYL 1066-45-1
8 ★	0.26	13.0	588	C3H9N1	I-PROPYLAMINE 75-31-0
9 ★	0.15	13.0	588	224 C3H9N1	METHYLETHYLAMINE 624-78-2
360 ★	0.48	13.0	588	224 C3H9N1	PROPYLAMINE 107-10-8
1 ★	0.16	2.7	547	340 C3H9N1	TRIMETHYLAMINE 75-50-3
2 ★	-0.96		510	C3H9N1O1	2-PROPANOL, 1-AMINO 78-96-6
3 ★	-0.94	13.0	579	C3H9N1O1	ETHANOLAMINE, N-METHYL 109-83-1
4 ★	-1.12	13.0	594	C3H9N1O1	PROPANOL, 3-AMINO 156-87-6
65 ★	-1.57	1394		C3H9N3O1	4,4-DIMETHYLSEMICARBAZIDE 22718-51-0
6 ★	-1.82	1394		C3H9N3O1	4-ETHYLSEMICARBAZIDE 13050-41-4
7 ★	-0.30	594	400	C3H9N3S1	4,4-DIMETHYLTHIOSEMICARBAZIDE 6926-58-5
8	-0.60	2182	459	C3H9O2P1	METHYLPHOSPHINIC ACID, ETHYL ESTER 16391-07-4
9 ★	-0.66	579		C3H9O3P1	METHYLPHOSPHONIC ACID, DIMETHYL ESTER 756-79-6
370	-0.52	508		C3H9O4P1	PHOSPHORIC ACID, TRIMETHYL ESTER 512-56-1
1	-0.78	547		C3H9O4P1	TRIMETHYLPHOSPHATE
2 ★	-0.07	600		C3H10N1O2P1S1	O,S-DIME-N-ME-PHOSPHORAMIDOTHIOATE 28187-49-9
3 ★	-1.43	13.0	579	C3H10N2	1,3-PROPANDIAMINE 109-76-2
4 ★	4.78	1179		C4Cl6	HEXACHLORO-1,3-BUTADIENE 67-68-3
75 ★	3.53	1814	459	C4H2Br2S1	2,3-DIBROMOTHIOPHENE 3140-93-0
6 ★	1.15	2499		C4H2Cl1F1N2	PYRAZINE, 2-CHLORO-6-FLUORO
7 ★	1.58	2499		C4H2Cl2N2	PYRAZINE, 2,5-DICHLORO
8 ★	1.53	2499		C4H2Cl2N2	PYRAZINE, 2,6-DICHLORO
9 ★	0.74	2499		C4H2F2N2	PYRAZINE, 2,6-DIFLUORO
380 ★	-0.25	594		C4H2N2	FUMARONITRILE 764-42-1
1 ✓	-2.70	1966		C4H3Au1O4S1.(Na1)2	GOLD SODIUM THIOMALONATE
2 ★	0.66	2412		C4H3Br1N2	5-BROMOPYRIMIDINE 4595-59-9
3 ★	0.93	2412		C4H3Br1N2	PYRAZINE, 2-BROMO
4 ★	0.50	2613		C4H3Br1N2	PYRIMIDINE, 2-BROMO
85 ★	-0.21	536		C4H3Br1N2O2	5-BROMOURACIL 51-20-7
6 ★	2.18	1055		C4H3Br1O1	3-BROMOFURAN 22037-28-1
7 ★	2.75	1478		C4H3Br1S1	2-BROMOTHIOPHENE 1003-09-4
8 ★	2.62	1478		C4H3Br1S1	3-BROMOTHIOPHENE 872-31-1
9 ★	0.29	579		C4H3Cl1N2	2-CHLOROPYRIMIDINE 1722-12-8
390 ★	0.70	2412		C4H3Cl1N2	PYRAZINE, 2-CHLORO
1 ★	0.10	2412		C4H3Cl1N2	PYRIDAZINE, 3-CHLORO 1120-95-2
2 ★	0.47	2412		C4H3Cl1N2	PYRIMIDINE, 4-CHLORO
3 ★	0.47	2412		C4H3Cl1N2	PYRIMIDINE, 5-CHLORO 17180-94-8
4 ★	-0.35	536		C4H3Cl1N2O2	5-CHLOROURACIL 1820-81-1
95 ★	2.54	1478		C4H3Cl1S1	2-CHLOROTHIOPHENE 96-43-5
6 ★	0.29	2412		C4H3F1N2	PYRAZINE, 2-FLUORO
7 ★	0.02	2412		C4H3F1N2	PYRIMIDINE, 2-FLUORO
8 ★	-0.03	2412		C4H3F1N2	PYRIMIDINE, 5-FLUORO 475-21-8
9	-0.99	7.4	401	1 C4H3F1N2O2	5-FLUOROURACIL 51-21-8 <i>antineoplastic</i>
400	-0.96	7.4	2270	1	5-FLUOROURACIL
1 ★	-0.89	7.4	401	2	5-FLUOROURACIL
2	-0.82	7.2	1797	314	5-FLUOROURACIL
3 ★	1.94	579	400	C4H3F7O1	BUTANOL, 2,2,3,3,4,4,4-HEPTAFLUORO 375-01-9
4 ★	0.04	536		C4H3I1N2O2	5-IODOURACIL 696-07-1
5 ★	-0.29	572		C4H3N1O2	MALEIMIDE 541-59-3
6 ★	1.55	1478		C4H3N1O2S1	2-NITROTHIOPHENE 609-40-5
7 ★	1.55	1478		C4H3N1O2S1	3-NITROTHIOPHENE 622-84-4
8 ★	0.66	594		C4H3N1O3	FURAN, 2-NITRO 609-39-2
9 ★	0.24	547		C4H3N3	4-CYANOPYRAZOLE 31108-57-3
410 ★	-1.97	1200	460	C4H3N5O1	8-AZAHYPOXANTHINE
1 ★	0.33	2387		C4H4Br1N3O2	IMIDAZOLE, 1-METHYL-2-BROMO-4-NITRO 16681-63-3
2 ★	0.77	2387		C4H4Br1N3O2	IMIDAZOLE, 1-METHYL-4-BROMO-5-NITRO 59177-47-6
3 ★	0.36	2387		C4H4Br1N3O2	IMIDAZOLE, 1-METHYL-4-NITRO-5-BROMO 933-67-9
4 ★	0.86	2387		C4H4Br1N3O2	IMIDAZOLE, 2-BROMO-4-NITRO-5-METHYL
15 ★	1.14	2387		C4H4Br1N3O2	IMIDAZOLE, 2-METHYL-4-NITRO-5-BROMO 933-67-9
6 ★	0.35	1519	400	C4H4Cl1N3	3-CL-6-PYRIDAZINEAMINE
7 ★	0.67	2499		C4H4Cl1N3	PYRAZINE, 2-AMINO-5-CHLORO
8 ★	0.95	2499		C4H4Cl1N3	PYRAZINE, 2-AMINO-6-CHLORO
9 ★	0.30	1008	354	C4H4Cl1N3O2	1-METHYL-4-NITRO-5-CHLOROIMIDAZOLE 4897-25-0
420 ★	0.19	2387		C4H4Cl1N3O2	IMIDAZOLE, 1-METHYL-2-CHLORO-4-NITRO 63634-21-9
1 ★	0.82	2387		C4H4Cl1N3O2	IMIDAZOLE, 1-METHYL-2-CHLORO-5-NITRO 86072-07-3
2 ★	0.89	2387		C4H4Cl1N3O2	IMIDAZOLE, 1-METHYL-4-CHLORO-5-NITRO 4897-31-8
3 ★	1.06	2387		C4H4Cl1N3O2	IMIDAZOLE, 2-METHYL-4-NITRO-5-CHLORO 4897-25-0
4 ★	2.01	594	400	C4H4Cl2	2-BUTYNE, 1,4-DICHLORO 821-10-3
25 ★	2.15	871		C4H4F6N2O1	N-NITROSO-BIS(2,2,2-TRIFLUOROETHYL)AMINE
6 ★	1.00	7.4	1975	1 C4H4I1N3O2	IMIDAZOLE, 1-METHYL-4-NITRO-5-IODO 35661-63-1
7 ★	1.29	7.4	1975	1 C4H4I1N3O2	IMIDAZOLE, 1-METHYL-5-NITRO-4-IODO 76529-47-0
8 ★	-0.23	924	400	C4H4N2	PYRAZINE 290-37-9
9 ★	-0.72	547		C4H4N2	PYRIDAZINE 289-80-5

## Exploring QSAR: Hydrophobic, Electronic, and Steric Constants

	logP	pH	Ref.	Note	MF	Name / CAS / activity	
430	★	-0.40	507		C4H4N2	PYRIMIDINE 289-05-2	
1	★	-0.99	2089		C4H4N2	SUCCINODINITRILE 110-61-2	
2	✓	-1.76	590	815	C4H4N2O1	2-PYRIMIDONE 557-01-7	
3	★	-1.82	924	400	"	2-PYRIMIDONE	
4	★	-1.38	924		C4H4N2O1	4-PYRIMIDONE 4562-27-0	
35	★	-1.49	924		C4H4N2O1	PYRAZINE-2-ONE 6270-63-9	
6	★	0.54	1625		C4H4N2O1S1	FORMAMIDE,N-2-THIAZOLYL 25602-39-5	
7	★	-0.28	536		C4H4N2O1S1	THIOURACIL 141-90-2 anti-anginal, thyroid inhibitor	
8	★	-0.84	570	815	C4H4N2O2	MALEIC ACID HYDRAZIDE 123-33-1 herbicide-growth regulator	
9	★	-1.07	536		C4H4N2O2	URACIL 66-22-8	
440	-1.00	7.2	1797	314	"	URACIL	
1	★	-1.47	505		C4H4N2O3	BARBITURIC ACID 67-52-7	
2	★	1.02	2168		C4H4N2O3	FURAZAN-2-OXIDE,2-METHYL-3-CARBOXALDEHYDE	
3	★	1.29	2168		C4H4N2O3	FURAZAN-2-OXIDE,3-CARBOXALDEHYDE-4-METHYL	
4	★	-1.66	527		C4H4N2O4	3-CARBOXYMETHYLSYDNE 26537-53-1	
45	★	-1.11	924	400	C4H4N2S1	2-(1H)-PYRIMIDINTHIONE 1450-85-7	
6	✓	-0.97	590	815	"	2-(1H)-PYRIMIDINTHIONE	
7	✓	-0.97	590		C4H4N2S1	PYRIMIDINE,2-THIOL	
8	★	0.04	871		C4H4N4O1	N-NITROSO-BIS(CYANOMETHYL)AMINE	
9	★	-0.17	2387		C4H4N4O4	IMIDAZOLE,1-METHYL-2,4-DINITRO 5213-50-3	
450	★	0.41	2387		C4H4N4O4	IMIDAZOLE,1-METHYL-4,5-DINITRO 19183-15-4	
1	★	0.77	2387		C4H4N4O4	IMIDAZOLE,2-METHYL-4,5-DINITRO 19183-16-5	
2	★	-0.96	1200		C4H4N6	8-AZAADENINE 1123-54-2	
3	★	-0.71	4.2	401	C4H4N6O1	8-AZAGUANINE 134-58-7 antineoplastic	
4	★	1.34	547	400	C4H4O1	FURAN 110-00-9	
55	★	-0.60	579		C4H4O2	2(5H)-FURANONE 497-23-4	
8	★	0.46	1.0	584	C4H4O4	FUMARIC ACID 110-17-8	
7	★	-0.34	1.0	584	C4H4O4	MALEIC ACID 110-16-7	
8	★	1.81	502		C4H4S1	THIOPHENE 110-02-1	
9	★	2.39	599		C4H5Cl3O2	ETHYLTRICHLOROACETATE	
460	★	1.18	505		C4H5F3O2	ACETIC ACID,TRIFLUORO-ETHYL ESTER 383-63-1	
1	★	0.40	1898		C4H5N1	ALLYLNITRILE 109-75-1	
2	★	0.29	579		C4H5N1	CYCLOPROPYLCYANIDE 5500-21-0	
3	★	0.68	1898		C4H5N1	METHACRYLONITRILE 126-98-7	
4	★	0.75	503		C4H5N1	PYRROLE 109-97-7	
65	★	0.45	594		C4H5N1O1	ISOXAZOLE,5-METHYL 5765-44-6	
6	★	0.46	1.0	342	C4H5N1O2	3-HYDROXY-5-METHYLISOXAZOLE 10004-44-1 fungicide	
7	★	-0.47	594		C4H5N1O2	CYANOACETIC ACID,METHYL ESTER 105-34-0	
8	★	0.97	594		C4H5N1S1	THIAZOLE,4-METHYL 693-95-8	
9	★	-0.07	163	459	C4H5N3	2-AMINOPYRAZINE 5049-61-6	
470	★	-0.53	2412		C4H5N3	PYRIDAZINE,4-AMINO 20744-39-2	
1	★	-0.22	505		C4H5N3	PYRIMIDINE,2-AMINO 5469-70-5	
2	★	-0.25	2412		C4H5N3	PYRIMIDINE,4-AMINO 591-54-8	
3	★	-0.89	924	400	C4H5N3O1	2-AMINO-4-PYRIMIDONE 108-53-2	
4	★	-2.40	7.2	314	C4H5N3O1	CYTOSINE 71-30-7	
75	★	-1.73	536		"	CYTOSINE	
6	★	0.74	7.4	1094	1	C4H5N3O1S1	2-METHYL-1,3,4-THIAZADIAZOLE-5-CARBOXALDOXIME
7	★	0.78	7.4	1094	2	"	2-METHYL-1,3,4-THIAZADIAZOLE-5-CARBOXALDOXIME
8	★	0.72	7.4	1094	1	C4H5N3O1S1	3-METHYL-1,3,4-THIAZADIAZOLE-5-CARBOXALDOXIME 61444-96-0
9	★	1.29	7.4	1094	2	"	3-METHYL-1,3,4-THIAZADIAZOLE-5-CARBOXALDOXIME
480		0.47	7.6	1769	212	C4H5N3O2	1,2,4-OXADIAZOLE-3-METHYL-5-HYDROXIMIC ACID 90507-21-4
1	★	0.55	7.4	2286	2	"	1,2,4-OXADIAZOLE-3-METHYL-5-HYDROXIMIC ACID
2	★	0.30	2186		C4H5N3O2	1,2,5-OXADIAZOLE,3-METHYL-4-CARBOXAMIDO	
3	★	1.02	2196		C4H5N3O2	1-(H)-PYRAZOLE,3-METHYL-4-NITRO 5334-39-4	
4	★	0.33	1731		C4H5N3O2	2-METHYL-5-NITROIMIDAZOLE	
85	★	0.06	1006	354	"	2-METHYL-5-NITROIMIDAZOLE 696-23-1	
6	★	0.10	7.4	2206	306	"	2-METHYL-5-NITROIMIDAZOLE
7	★	0.18	7.4	2206	306	C4H5N3O2	4-METHYL-5-NITROIMIDAZOLE 14003-66-8
8	★	-0.17	2387		C4H5N3O2	IMIDAZOLE,1-METHYL-2-NITRO 1671-82-5	
9	★	-0.44	2387		C4H5N3O2	IMIDAZOLE,1-METHYL-4-NITRO 3034-41-1	
490	★	0.16	7.4	2206	306	C4H5N3O2	IMIDAZOLE,1-METHYL-5-NITRO 3034-42-2
1	★	0.13	2387		C4H5N3O2	IMIDAZOLE,2-METHYL-4-NITRO	
2	★	0.23	2387		C4H5N3O2	IMIDAZOLE,4-NITRO-5-METHYL	
3	★	0.03	2166		C4H5N3O3	FURAZAN-2-OXIDE,3-METHYL-4-CARBOXAMIDO	
4	★	0.36	2166		C4H5N3O3	FURAZAN-2-OXIDE,4-METHYL-3-CARBOXAMIDO	
95	★	0.13	2387		C4H5N3O3	IMIDAZOLE,4-NITRO-5-METHOXY 68019-78-3	
6	★	1.99	547	400	C4H6	1,3-BUTADIENE 106-99-0	
7	★	1.46	547	400	C4H6	2-BUTYNE 503-17-3	
8	★	0.56	1896		C4H6Cl1N1	4-CHLOROBUTYRONITRILE 628-20-6	
9	★	0.83	871		C4H6Cl2N2O1	3,4-DICHLORO-N-NITROSPYRROLIDINE 59863-59-1	
500	★	0.87	594		C4H6F2O2	DIFLUOROACETIC ACID,ETHYL ESTER 454-31-9	
1	★	0.23	8.0	547	1	C4H6N2	4-METHYLIMIDAZOLE 822-36-6
2	★	-0.06	8.4	579	1	C4H6N2	IMIDAZOLE,1-METHYL 616-47-7
3	★	0.24	594		C4H6N2	IMIDAZOLE,2-METHYL 693-98-1	
4	★	0.23	594	400	C4H6N2	PYRAZOLE,1-METHYL 930-36-9	
5	★	0.37	547		C4H6N2O1	4-METHOXYPYRAZOLE	
6	★	0.26	871		C4H6N2O1	DELTA-3-N-NITROSPYRROLIDINE 10552-94-0	
7	★	0.71	2166		C4H6N2O1	FURAZAN,DIMETHYL 4975-21-7	
8	★	0.23	2166		C4H6N2O2	FURAZAN,DIMETHYL,2-OXIDE 2518-42-5	
9	★	-2.39	7.0	1207	1	C4H6N2O2	MUSCIMOL 2763-96-4 agonist-gabba-a
510	★	1.28	2166		C4H6N2S1	1,2,5-THIAZADIAZOLE,3,4-DIMETHYL	
1	★	0.03	547		C4H6N2S1	2,5-DIMETHYL-1,3,4-THIAZADIAZOLE 27464-82-0	
2	★	-0.34	599		C4H6N2S1	METHIMAZOLE 60-56-0 thyroid inhibitor	
3	★	0.69	2166		C4H6N2Se1	1,2,5-SELENODIAZOLE,3,4-DIMETHYL	
4	★	-0.45	2499		C4H6N4	PYRAZINE,2,6-DIAMINO	

	logP	pH	Ref.	Note	MF	Name / CAS / activity	
15	★	-1.10	9.0	594	1	C4H8N4O1	4-IMIDAZOLECARBOXAMIDE,5-AMINO
6	★	0.38		57		C4H8N4O1S1	3-METHYLTHIO-4-AMINO-1,2,4-TRIAZINE-5-ONE
7	★	-0.19		2592		C4H8N4O2	1,2,4-TRIAZOLE,1-ETHYL-3-NITRO
8	★	-0.23		2166		C4H8N4O2	1,2,5-OXADIAZOLE,3-AMINO-4-ACETYLAMINO
9		-1.00		2387		C4H8N4O2	IMIDAZOLE,1-METHYL-4-NITRO-5-AMINO 4531-54-8
520	★	-1.26	7.4	830	1	C4H8N4O2	N-DIAZOACETYLGLYCINEAMIDE 817-99-2
1	★	-0.45	7.2	2036	1	C4H8N4O3S2	ACETAZOLAMIDE 59-66-5 carbonic anhydrase inhibitor
2	★	-0.26		505		"	ACETAZOLAMIDE
3	★	-0.74		2279		C4H8N4O4S1	IMIDAZOLE,1-METHYL-4-NITRO-5-SULFONAMIDO 6339-55-5
4	★	0.46		547	400	C4H6O1	2,5-DIHYDROFURAN 1708-29-8
25	★	0.60		589		C4H6O1S1	G-THIOBUTYROLACTONE 39700-44-2
6	★	-1.34		541		C4H6O2	2,3-BUTANEDIONE 431-03-8
7	★	0.80		1402		C4H6O2	ACRYLIC ACID,METHYL ESTER 96-33-3
8	★	0.72		300		C4H6O2	CROTONIC ACID 3724-65-0
9	★	0.63	1.0	579	342	C4H6O2	CYCLOPROPANECARBOXYLIC ACID 1759-53-1
530	★	-0.52		594		C4H6O2	ERYTHRITOLANHYDRIDE 564-00-1
1	★	-0.64		547		C4H6O2	G-BUTYROLACTONE 96-48-0
2	★	0.93		997		C4H6O2	METHACRYLIC ACID 79-41-4
3	★	0.73		572		C4H6O2	VINYLAETATE 108-05-4
4	★	-0.41		599		C4H6O3	PROPYLENECARBONATE 108-32-7 gelling agent
35	★	-0.17		579		C4H6O4	OXALIC ACID,DIMETHYL ESTER 553-90-2
6	★	-0.59		510		C4H6O4	SUCCINIC ACID 110-15-6
7	★	-0.57	7.4	2288	1	"	SUCCINIC ACID
8	★	-1.26		510		C4H6O5	MALIC ACID 6915-15-7 pharmaceutical acid
9		1.11		1966	459	C4H7Au1Cl1N1	I-PROPYLSOCYANIDE GOLD CHLORIDE
540		2.53		1560	459	C4H7Br1	4-BROMO-1-BUTENE 5162-44-7
1		1.11		1560	459	C4H7Br1O2	2-BROMOETHYLACETATE 927-68-4
2	★	1.42		510		C4H7Br1O2	A-BROMOBUTYRIC ACID 80-58-0
3		1.38		600		C4H7Br2Cl2O4P1	NALED 300-76-5 insecticide
4	★	0.94	5.0	590		C4H7Cl1O2	CHLOROACETIC ACID,ETHYL ESTER 105-39-5
45	★	1.40		51		C4H7Cl2O3P1	DICHLOROVINYLPHOSPHONATE,O,O-DIMETHYL 1185-97-3
6	★	1.43		2049		C4H7Cl2O4P1	DICHLOROVINYLPHOSPHATE,O,O-DIMETHYL 62-73-7 anthelmintic-insecticide
7	★	2.03		505		C4H7Cl3O1	CHLOROBUTANOL 57-15-8 analgesic (dental), antimicrobial
8	★	1.04		1942		C4H7F3O1	3,3,3-TRIFLUORO-2-METHYLPROPANOL-2
9	★	0.71		1942		C4H7F3O1	4,4,4-TRIFLUOROBUTANOL-2
550	★	0.90		1942		C4H7F3O1	4,4,4-TRIFLUOROBUTANOL
1	★	0.53		1896		C4H7N1	BUTYRONITRILE 109-74-0
2	★	0.46		1896		C4H7N1	I-BUTYRONITRILE 78-82-0
3	★	-0.85	5.0	2425	1	C4H7N1O1	2-PYRROLIDINONE 618-46-5
4	★	-2.84		2654	448	C4H7N1O2	AZACYCLOBUTANE,A-CARBOXYLIC ACID
55	★	-2.78		2654	448	C4H7N1O2	CYCLOPROPANECARBOXYLIC ACID,A-AMINO
8	★	1.21	7.8	2334		C4H7N1O2S1	2-OXOPROPANAL OXIME,1-METHYLTHIO 112740-61-1
7	★	-1.02	7.8	2334	1	C4H7N1O3S1	2-OXOPROPANAL OXIME,1-METHYLSULFOXIDE 112740-56-4
8	★	-0.72	7.8	2334	2	"	2-OXOPROPANAL OXIME,1-METHYLSULFOXIDE
9	★	-4.25		1590	459	C4H7N1O4	ASPARTATE,MONOSODIUM SALT
560		-0.84	7.8	2334	1	C4H7N1O4S1	2-OXOPROPANAL OXIME,1-METHYLSULFONE 112740-58-6
1	★	-0.69	7.8	2334	2	"	2-OXOPROPANAL OXIME,1-METHYLSULFONE
2	★	-0.05		561		C4H7N1S1	2-AZACYCLOPENTANTHIONE 2295-35-4
3	★	-0.30		1137		C4H7N3O1	2-AMINO-5-ETHYL-1,3,4-OXADIAZOLE
4	★	-1.78	7.4	1010	1	C4H7N3O1	CREATININE 60-27-5
65		-0.76	7.4	830	1	C4H7N5O2	N-DIAZOACETYLGLYCINE HYDRAZIDE 820-75-7
6	★	2.40		547	400	C4H8	1-BUTENE 106-98-9
7	★	2.33		547	400	C4H8	2-BUTENE-CIS 590-18-1
8	★	2.31		547	400	C4H8	2-BUTENE-TR 624-84-6
9	★	2.34		547	400	C4H8	I-BUTYLENE 115-11-7
570	★	0.34		507		C4H8Br1N1O1	BROMOACETAMIDE,N-ETHYL
1	★	1.29		579		C4H8Cl2O1	2,2-DICHLOROETHYLETHYL 111-44-4
2	★	0.51		51		C4H8Cl3O4P1	DIME-1-OH-2,2,2-TRICLLETHYLPHOSPHONATE 52-68-6 anthelmintic (vet)
3	★	1.06		1701		C4H8F3N1	N,N-DIMETHYL-2,2,2-TRIFLUOROETHYLAMINE 819-06-7
4	★	0.74		1701		C4H8F3N1	N-ETHYL-2,2,2-TRIFLUOROETHYLAMINE
75	★	0.52		507		C4H8N2	2-IMIDAZOLINE,2-METHYL 534-26-9
6	★	-0.19		871		C4H8N2O1	N-NITROSPYRROLIDINE 930-55-2
7	★	0.40		871		C4H8N2O1S1	N-NITROSOTHIOMORPHOLINE 26541-51-5
8	★	-0.80		599		C4H8N2O2	1-DIMETHYLAMINO-2-NITROETHYLENE
9	★	-1.83	7.1	1591		C4H8N2O2	GLYCIN-AMIDE,N-ACETYL
580		-1.68	7.0	2309	1	"	GLYCIN-AMIDE,N-ACETYL
1	★	-0.70		2198		C4H8N2O2	METHYLUREA,N-ACETYL 623-59-6
2	★	-0.44		871		C4H8N2O2	N-NITROSOMORPHOLINE 59-89-2
3	★	-3.41		1591		C4H8N2O3	ASPARAGINE 70-47-3
4	★	-2.92		547		C4H8N2O3	GLYCINE,GLYCYL 556-50-3
85	★	-0.68		1157		C4H8N2S1	N,N'-TRIMETHYLENETHIOUREA 2055-46-1
6	★	-0.40		1173	537	C4H8N4	1,3-DIMETHYL-2-CYANOQUANIDINE
7	★	0.51		2166		C4H8N4O1	1,2,5-OXADIAZOLE,3-AMINO-4-ETHYLAMINO
8	★	-0.85		871		C4H8N4O2	N,N'-DINITROSOPIPERAZINE 140-79-4
9	★	0.29		503		C4H8O1	2-BUTANONE 78-93-3
590	★	0.88	7.4	547	1	C4H8O1	BUTYRALDEHYDE 123-72-8
1	★	1.04		530		C4H8O1	ETHYL VINYL ETHER 109-92-2
2	★	0.48		547	400	C4H8O1	TETRAHYDROFURAN 109-99-9
3	★	-0.81		594		C4H8O2	2-BUTENE-1,4-DIOL 110-64-5
4	★	0.73		503		C4H8O2	ACETIC ACID,ETHYL ESTER 141-78-6
95	★	0.79		510		C4H8O2	BUTYRIC ACID 107-92-6
6	★	-0.27		547	400	C4H8O2	DIOXANE 123-91-1
7	★	0.83		508		C4H8O2	FORMIC ACID,PROPYL ESTER 110-74-7
8	★	1.10	3.5	2391	1	C4H8O2	I-BUTYRIC ACID 79-31-2
9	★	0.11		2596		C4H8O2	METHYL GLYCIDYL ETHER 930-37-0



	logP	pH	Ref.	Note	MF	Name / CAS / activity
600	★	0.82	579	400	C4H8O2	PROPIONIC ACID, METHYL ESTER 554-12-1
1	✓	-3.20	508		C4H8O2	SODIUM BUTYRATE
2	★	-0.77	572		C4H8O2S1	TETRAHYDROTHIOPHENE-, 1,1-DIOXIDE 126-33-0
3	★	-0.36	510		C4H8O3	A-HYDROXY-I-BUTYRIC ACID 594-61-6
4	★	2.75	1560	100	C4H9Br1	1-BROMOBUTANE 109-65-9
5	★	1.15	594	400	C4H9Br1	PROPANE, 2-BROMO-2-METHYL 507-19-7
6	★	2.64	547	60	C4H9Cl1	1-CHLOROBUTANE 109-69-3
7	★	2.33	594	400	C4H9Cl1	BUTANE, 2-CHLORO 78-66-4
8	★	1.82	579	400	C4H9Cl1	T-BUTYL CHLORIDE 507-20-0
9	★	0.98	579		C4H9Cl1O1	2-CHLOROETHYLETHER 628-34-2
610	★	0.85	590		C4H9Cl1O1	BUTANOL, 4-CHLORO 928-51-8
1		0.41	2019		C4H9Cl3Sn1	TRICHLOROSTANNANE, BUTYL 1118-46-3
2	★	2.58	579	60	C4H9F1	1-FLUOROBUTANE 2366-52-1
3	★	-1.60	2084		C4H9Hg1N1O2S1	CYSTEINE, S-METHYL MERCURY
4	★	0.46	588	224	C4H9N1	PYRROLIDINE 123-75-1
15	★	-0.21	503		C4H9N1O1	BUTYRAMIDE 541-35-5
6	★	-0.86	547		C4H9N1O1	MORPHOLINE 110-91-8
7	★	-0.77	536		C4H9N1O1	N,N-DIMETHYLACETAMIDE 127-19-5
8	★	1.47	547	400	C4H9N1O2	1-NITROBUTANE 627-05-4
9	★	1.17	535		C4H9N1O2	2-METHYL-2-NITROPROPANE 594-70-7
620	★	1.20	2571		C4H9N1O2	2-NITROBUTANE 600-24-8
1	★	-2.53	2654	448	C4H9N1O2	A-AMINOBUTYRIC ACID 50-60-4
2	★	-2.48	2323	468	"	A-AMINOBUTYRIC ACID
3	★	-3.17	1207	1	C4H9N1O2	G-AMINOBUTYRIC ACID 56-12-2
4	★	-2.91	2654	448	C4H9N1O2	GLYCINE, N,N-DIMETHYL 1118-68-9
25	★	1.40	2571		C4H9N1O2	ISO-NITROBUTANE 625-74-1
6	★	0.34	572		C4H9N1O2	N-METHYL CARBAMIC ACID, ETHYL ESTER 105-40-8
7	★	0.38	172	1	C4H9N1O2	O-PROPYL CARBAMATE 627-12-3
8	★	2.15	536		C4H9N1O3	BUTYL NITRATE 928-45-0
9	★	-2.94	1207	1	C4H9N1O3	THREONINE 72-19-5 amino acid
630	★	-1.55	1394		C4H9N3O1	4-ALLYLSEMICARBAZIDE 57421-73-5
1	★	0.18	871		C4H9N3O1	N-NITROSOPIPERAZINE 5632-47-3
2	★	0.36	871		C4H9N3O2	1-NITROSO-TRIMETHYLUREA 3475-63-6
3	★	0.30	979	364	C4H9N3O2	1-PROPYL-1-NITROSOUREA 816-57-9
4	★	2.89	547	400	C4H10	BUTANE 106-97-8
35	★	2.76	547	400	C4H10	I-BUTANE 78-28-5
6	★	-3.15	2019		C4H10Cl2Sn1	DICHLOROSTANNANE, DIETHYL 868-55-7
7	★	-0.85	1027		C4H10N1O3P1S1	ORTHENE 30560-19-1 insecticide
8	★	-1.50	594		C4H10N2	PIPERAZINE 110-85-0 anthelmintic
9	★	-0.62	1137		C4H10N2O1	BUTYRIC ACID HYDRAZIDE 3538-65-6
640	★	-0.63	1137		C4H10N2O1	I-BUTYRIC ACID HYDRAZIDE 3619-17-8
1	★	0.48	871		C4H10N2O1	N-NITROSODIETHYLAMINE 55-19-5
2	★	0.51	2570		C4H10N2O1	N-NITROSOMETHYLPROPYL AMINE 924-46-9
3	★	0.20	1184	1	C4H10N2O2	3-I-PROPYLHYDROXYUREA 60165-07-3
4	★	-0.22	1184	1	C4H10N2O2	3-PROPYLHYDROXYUREA 5710-12-3
45	✓	-4.64	2323	468	C4H10N2O2	BUTYRIC ACID, 2,4-DIAMINO 305-82-4
6	★	0.10	579		C4H10N2S1	THIOUREA, TRIMETHYL 2489-77-2
7	★	0.88	2306	1	C4H10O1	BUTANOL 71-36-3
8	★	0.88	532		"	BUTANOL
9	★	0.89	547	400	C4H10O1	ETHYLETHER 60-29-7 anesthetic
650	★	0.76	425		C4H10O1	I-BUTANOL 78-83-1
1	★	1.21	594	400	C4H10O1	METHYLPROPYLETHER 557-17-5
2	★	0.61	503		C4H10O1	S-BUTANOL 78-92-2
3	★	0.35	547	400	C4H10O1	T-BUTANOL 75-65-0
4	★	-0.83	579	400	C4H10O2	1,4-BUTANEDIOL 110-63-4
55	★	-0.92	510		C4H10O2	2,3-BUTANEDIOL 513-85-9
6	★	-0.21	1819		C4H10O2	ETHANE, 1,2-DIMETHOXY 110-71-4
7	★	-0.32	2562		C4H10O2	ETHOXYETHANOL 110-80-5
8	★	-0.59	594		C4H10O2S1	DIETHYLSULFONE 597-35-3
9	★	-0.63	594	400	C4H10O2S1	THIODIGLYCOL 111-48-8
660	★	0.25	578	224	C4H10O3	TRIMETHYLOROTHOFORMATE 149-73-5
1	★	-2.29	1087		C4H10O4	ERYTHRITOL 149-32-6
2	★	1.14	579		C4H10O4S1	DIETHYLSULFATE 64-67-5
3	★	2.28	536		C4H10S1	BUTANETHIOL 109-79-5
4	★	1.95	503		C4H10S1	DIETHYL SULFIDE 352-93-2
65	★	-1.22	834	1	C4H11N1	BUTYLAMINE 109-73-9
6	★	0.97	588	224	"	BUTYLAMINE
7	★	0.58	588	224	C4H11N1	DIETHYLAMINE 109-89-7
8	★	0.70	567		C4H11N1	ETHANAMINE, N,N-DIMETHYL 598-56-1
9	★	0.73	588	224	C4H11N1	I-BUTYLAMINE 78-81-9
670	★	0.84	579		C4H11N1	METHYLPROPYLAMINE 627-35-0
1	★	0.74	588	224	C4H11N1	S-BUTYLAMINE 513-49-5
2	★	0.40	505		C4H11N1	T-BUTYLAMINE 75-64-9
3	★	-1.43	510		C4H11N1O2	DIETHANOLAMINE 111-42-2
4	★	-1.30	1394		C4H11N3O1	4-ISOPROPYLSEMICARBAZIDE 57930-20-8
75	★	-1.10	1394		C4H11N3O1	4-PROPYLSEMICARBAZIDE 57421-72-4
6	★	-1.43	761	314	C4H11N5	N,N-DIMETHYLBIGUANIDE 657-24-9 antidiabetic
7	★	3.31	547		C4H12Ge1	TETRAMETHYLGERMANE 865-52-1
8	★	0.15	600		C4H12N1O2P1S1	O,S-DIETHYLPHOSPHORAMIDOTHIOATE 16271-10-6
9	★	0.07	600		C4H12N1O2P1S1	O,S-DIME-N-ET-PHOSPHORAMIDOTHIOATE 52067-48-8
680	★	-3.92	2173		C4H12N1.I1	TETRAMETHYL AMMONIUM IODIDE
1	★	-2.52	1901	820	"	TETRAMETHYL AMMONIUM IODIDE
2	★	-0.82	594		C4H12N2	1,2-ETHANDIAMINE, N,N'-DIMETHYL 110-70-3
3	★	-2.66	1010	1	C4H12N2	TETRAMETHYLENEDIAMINE 110-80-1
4	★	2.97	547		C4H12Pb1	TETRAMETHYLLEAD 76-74-1

	logP	pH	Ref.	Note	MF	Name / CAS / activity
85	★	3.24	594	400	C4H12Si1	TETRAMETHYLSILANE 75-76-3
6	★	3.48	547	400	C4H12Sn1	TETRAMETHYLtin 594-27-4
7	★	3.53	528	831	C5Cl5N1	2,3,4,5,6-PENTACHLOROPYRIDINE 2176-62-7
8	★	5.04	1736		C5Cl6	HEXACHLORO-1,3-CYCLOPENTADIENE
9	★	5.04	1369	459	C5Cl6	HEXACHLOROCYCLOPENTADIENE 77-47-4
690	★	2.34	579		C5F12	PERFLUOROPENTANE
1		4.40	579	400		PERFLUOROPENTANE
2	★	3.08	7.3	509	2 C5H1Br3N4	PURINE,2,6,8-TRIBROMO
3	★	3.90	7.3	509	2 C5H1Cl3N4	PURINE,2,6,8-TRICHLORO 2562-52-9
4	★	3.32	529	831	C5H1Cl4N1	2,3,5,6-TETRACHLOROPYRIDINE 2402-79-1
95	★	0.92	2499		C5H2Cl1N3	PYRAZINE,2-CHLORO-5-CYANO
6	★	0.79	2499		C5H2Cl1N3	PYRAZINE,2-CHLORO-6-CYANO
7	★	3.11	529	831	C5H2Cl3N1	2,3,5-TRICHLOROPYRIDINE 16063-70-0
8	★	2.77	529	831	C5H2Cl3N1	2,3,6-TRICHLOROPYRIDINE 6515-09-9
9	★	2.68	529	831	C5H2Cl3N1	2,4,6-TRICHLOROPYRIDINE 16063-69-7
700	★	3.21	1190		C5H2Cl3N1O1	3,5,6-TRICHLORO-2-PYRIDINOL 6515-38-4
1		3.21	1178		C5H2Cl3N1O1	3,5,8-TRICHLOROPYRIDINOL
2	★	2.11	529	831	C5H3Cl2N1	2,3-DICHLOROPYRIDINE 2402-77-9
3	★	2.40	529	831	C5H3Cl2N1	2,5-DICHLOROPYRIDINE 16110-09-1
4	★	2.15	529	831	C5H3Cl2N1	2,6-DICHLOROPYRIDINE 2402-78-0
5	★	2.56	529	831	C5H3Cl2N1	3,5-DICHLOROPYRIDINE 2457-47-8
6	★	1.17	594	400	C5H3F2N1	PYRIDINE,2,6-DIFLUORO 1513-65-1
7	★	0.04	536		C5H3F3N2O2	5-TRIFLUOROMETHYLRACIL 54-20-6
8	★	0.96	1478		C5H3N1O1	2-CYANOFURAN 617-90-3
9	★	1.01	594	1	C5H3N1O4	2-FURALDEHYDE,5-NITRO 698-63-5
710	★	-1.72	1008	354	C5H3N1O6	5-NITRO-2-FUROIC ACID
1	★	1.27	1478		C5H3N1S1	2-CYANTHIOPIHENE 1003-31-2
2	★	-0.01	2412		C5H3N3	PYRAZINE,2-CYANO
3	★	-0.63	2412		C5H3N3	PYRIDAZINE,4-CYANO
4	★	-0.31	2412		C5H3N3	PYRIMIDINE,2-CYANO
15	★	-0.08	2412		C5H3N3	PYRIMIDINE,4-CYANO 42839-04-3
6	★	-0.93	547	342	C5H3N3O2	5-CYANOURACIL 4425-56-3
7	★	1.42	260		C5H4Br1N1	2-BROMOPYRIDINE 109-04-6
8	★	1.60	260		C5H4Br1N1	3-BROMOPYRIDINE 626-55-1
9	★	1.54	260		C5H4Br1N1	4-BROMOPYRIDINE 1120-87-2
720	★	1.22	594	400	C5H4Cl1N1	2-CHLOROPYRIDINE 109-09-1
1		1.34	566	1	"	2-CHLOROPYRIDINE
2	★	1.33	163	459	C5H4Cl1N1	3-CHLOROPYRIDINE 626-60-8
3	★	1.28	2412		C5H4Cl1N1	4-CHLOROPYRIDINE 626-61-9
4	★	0.93	547		C5H4Cl1N1O1	PYRIDINE,2-CHLORO-6-HYDROXY
25	★	0.00	1519	400	C5H4Cl1N3O1	3-CHLORO-6-PYRIDAZINECARBOXAMIDE
6	★	0.28	2499		C5H4Cl1N3O1	PYRAZINE,2-CHLORO-6-CARBOXAMIDO
7	★	0.84	2412		C5H4F1N1	PYRIDINE,2-FLUORO 372-48-5
8	★	0.77	2412		C5H4F1N1	PYRIDINE,3-FLUORO 372-47-4
9	★	1.80	1519	459	C5H4I1N1	3-IODOPYRIDINE 1120-90-7
730	★	1.13	2221	400	C5H4N2	PYRROLE,2-CYANO 4513-94-4
1	★	0.48	163	459	C5H4N2O2	2-NITROPYRIDINE 15009-91-3
2	★	0.60	163	459	C5H4N2O2	3-NITROPYRIDINE 2530-26-9
3	★	0.33	570		C5H4N2O2	4-NITROPYRIDINE 1122-61-8
4	★	-0.74	547	1	C5H4N2O3	4-NITROPYRIDINE-1-OXIDE 1124-33-0
35	★	-0.57	7.0	452	1	"
6	★	-0.55	547		"	4-NITROPYRIDINE-1-OXIDE
7	★	-1.03	547		C5H4N2O3	5-FORMYLRACIL 1195-08-0
8	★	0.30	1731		C5H4N2O4	NIFUROXIME 6236-05-1 antibacterial (topical)
9	★	-1.70	2447	300	C5H4N2O4	OROTIC ACID 65-86-1 uricosuric
740	★	-0.37	547		C5H4N4	PURINE 120-73-0
1		-0.21	7.0	1793	1	"
2	★	-0.09	1627	400	C5H4N4	PURINE
3	★	-0.55	2070	306	C5H4N4O1	TETRAZOLO(1,5A)PYRIDINE 274-87-3
4	★	-1.11	283	1	C5H4N4O1	ALLOPURINOL 315-30-0 xanthine oxidase inhibitor
45	★	-0.73	572		C5H4N4O2	HYPOXANTHINE 68-94-0
6	★	-2.92	7.4	293	1	"
7	★	-2.90	7.4	1200	1	"
8	★	-2.17	1200	460	"	XANTHINE 69-89-6
9	★	0.18	2312	337	"	URIC ACID 69-83-2
750	★	0.01	7.4	401	2	"
1	★	1.01	1478		C5H4O1S1	URIC ACID
2	★	1.02	1478		C5H4O1S1	6-PURINETHIOL 60-44-2 antineoplastic
3	★	0.51	1478		C5H4O2	3-THIOPHENECARBOXALDEHYDE 498-62-4
4	★	0.41	572		C5H4O2	THIOPHENE-2-CARBOXALDEHYDE 98-03-3
55	★	1.50	1478		C5H4O2S1	FURAN-3-CARBOXALDEHYDE 498-60-2
6	★	1.57	1478		C5H4O2S1	FURFURAL 98-01-1
7	★	0.50	1937	459	C5H4O3	THIOPHEN-3-CARBOXYLIC ACID 88-13-1
8	★	1.03	1478		C5H4O3	THIOPHENE-2-CARBOXYLIC ACID 527-72-0
9	★	0.64	1055		C5H4O3	4-HYDROXY-2-PYRONE 675-10-5
760	★	-1.12	1584		C5H5Br1N2O3	FURAN-3-CARBOXYLIC ACID 486-93-7
1	★	1.08	2499		C5H5Cl1N2	FURANE-2-CARBOXYLIC ACID 88-14-2
2	★	1.03	2499		C5H5Cl1N2	PYRIMIDINE,2,4-DIONE,3-HYDROXY-5-BROMO-6-METHYL 77317-64-7
3	★	0.89	1519	459	C5H5Cl1N2O1	PYRAZINE,2-CHLORO-5-METHYL
4	★	1.52	2499		C5H5Cl1N2O1	PYRAZINE,2-CHLORO-6-METHYL
85	★	1.65	2499		C5H5Cl1N2O1	3-CHLORO-6-METHOXYPYRIDAZINE
6	★	-0.82	1375		C5H5Cl1N2O1	PYRAZINE,2-CHLORO-5-METHOXY
7	★	2.55	2506		C5H5Cl3N2O1S1	PYRIDAZINE,3-CHLORO-4-HYDROXY-6-METHYL
8	★	0.63	2362	1	C5H5F1N2	ETHAZOL 2593-15-9 fungicide
9	★	2.12	505		C5H5F5O2	PYRIDINE,3-FLUORO-4-AMINO
						PENTAFUOROPROPIONIC ACID,ETHYL ESTER 426-65-3

	logP	pH	Ref.	Note	MF	Name / CAS / activity
770	0.59		1734		C5H5N1	PYRIDINE,PENTADEUTERO 7291-22-7
1	0.60	7.2	2317	1	C5H5N1	PYRIDINE 110-86-1
2	0.65		502		"	PYRIDINE
3	0.48		572		C5H5N1O1	3-HYDROXYPYRIDINE 109-00-2
4	-1.31		590	815	C5H5N1O1	4-PYRIDONE 626-64-2
75	-1.30		924	400	"	4-PYRIDONE
8	-0.58		548	815	C5H5N1O1	A-PYRIDONE 109-10-4
7	-1.27	7.4	1940	1	C5H5N1O1	PYRIDINE,1-OXIDE 694-59-7
8	-1.20		2815		"	PYRIDINE,1-OXIDE
9	0.64		1625		C5H5N1O1	PYRROLE,2-CARBOXYALDEHYDE 1003-29-8
780	-0.11	7.0	332	1	C5H5N1O2	FURAN-2-CARBOXAMIDE 609-38-1
1	-0.11		1055		"	FURAN-2-CARBOXAMIDE
2	0.09		1478		C5H5N1O2	FURANE-3-CARBOXAMIDE 609-35-8
3	-0.61		594		C5H5N1O2	PYRIDINE-N-OXIDE,3-HYDROXY 6602-28-4
4	0.85	2.0	1625		C5H5N1O2	PYRROLE,2-CARBOXYLIC ACID 634-97-9
85	0.68		1348		C5H5N1O3	5-METHYLSOXAZOLE,3-CARBOXYLIC ACID 4867-42-5
6	-0.13		590	815	C5H5N1S1	2-PYRIDINETHIONE 2637-34-5
7	0.20		590	815	C5H5N1S1	4-PYRIDINETHIONE 4556-23-4
8	0.52		1478		C5H5N1S1	THIOPHEN-2-CARBOXAMIDE 5813-89-8
9	0.50		1478		C5H5N1S1	THIOPHEN-3-CARBOXAMIDE 51460-47-0
790	1.34		2221	457	C5H5N1S2	THIOPHENE,2-THIOCARBOXAMIDE 20300-02-1
1	-0.60		1519	400	C5H5N3O1	2-PYRAZINECARBOXAMIDE 98-98-4 <i>antibacterial (tuberculostatic)</i>
2	-0.59	7.2	2317	1	"	2-PYRAZINECARBOXAMIDE
3	-0.73		2412		C5H5N3O1	PYRIDAZINE,3-CARBAMOYL
4	-0.96		2412		C5H5N3O1	PYRIDAZINE,4-CARBAMOYL 68511-47-1
95	-1.20		2412		C5H5N3O1	PYRIMIDINE,2-CARBOXAMIDO
6	-0.88		2412		C5H5N3O1	PYRIMIDINE,4-CARBOXAMIDE
7	-0.92		2412		C5H5N3O1	PYRIMIDINE,5-CARBOXAMIDE 40829-49-5
8	-1.02		594		C5H5N3O2	2-PYRIDINEAMINE,N-NITRO 26482-54-2
9	0.65		2138	459	C5H5N3O2	PYRIDINE,2-AMINO-5-NITRO 4214-76-0
800	-0.69	9.0	1409		C5H5N3O3	5-NITROIMIDAZOLE,1-ME-2-FORMYL 4750-57-6
1	-0.10		2474		C5H5N3O3	IMIDAZOLE,5-CARBOXYALDEHYDE,1-METHYL-2-NITRO 38928-74-0
2	1.30		594		C5H5N3O3S1	NITHIAMIDE 140-40-9 <i>antibacterial,antiprotozoal (vet)</i>
3	-1.52	7.4	694	1	C5H5N3O4	1-B-CARBOXYMETHYL-5-NITROIMIDAZOLE, SODIUM SALT
4	-0.34		2474		C5H5N3O4	IMIDAZOLE-1-ACETIC ACID,2-NITRO
5	-0.34		1519	400	C5H5N3S1	PYRIMIDINE-2-THIOCARBOXAMIDE
6	-0.16	7.4	293	1	C5H5N5	ADENINE 73-24-5
7	-0.09		536		"	ADENINE
8	-0.05	7.4	2348	1	"	ADENINE
9	-0.96	7.4	594	1	C5H5N5O1	GUANINE 73-40-5
810	-0.07	8.2	401	2	C5H5N5S1	THIOGUANINE 154-42-7 <i>antineoplastic</i>
1	2.66		541		(C5H5)2Fe1	FERROCENE 102-54-5
2	0.87		2387		C5H6Br1N3O2	IMIDAZOLE,1,2-DIMETHYL-4-BROMO-5-NITRO
3	0.44		2387		C5H6Br1N3O2	IMIDAZOLE,1,2-DIMETHYL-4-NITRO-5-BROMO 21117-52-2
4	0.82		2387		C5H6Br1N3O2	IMIDAZOLE,1,4-DIMETHYL-2-BROMO-5-NITRO
15	0.39		2387		C5H6Br1N3O2	IMIDAZOLE,1,5-DIMETHYL-2-BROMO-4-NITRO
6	0.87		2387		C5H6Cl1N3O2	IMIDAZOLE,1,2-DIMETHYL-4-CHLORO-5-NITRO 91027-94-0
7	0.34		2387		C5H6Cl1N3O2	IMIDAZOLE,1,2-DIMETHYL-4-NITRO-5-CHLORO 91027-93-9
8	-0.21	7.4	2381	1	C5H6F2N4O3	TRIAZINE,3-NITRO-1-(3-HYDROXY-2,2-DIFLUORO)PROPYL
9	0.49		548	815	C5H6N2	2-AMINOPYRIDINE
820	0.49		548	815	"	2-AMINOPYRIDINE 504-29-0
1	0.23		163	459	C5H6N2	2-METHYLPYRAZINE 109-08-0
2	0.11		260		C5H6N2	3-AMINOPYRIDINE 462-06-8
3	-0.76	7.4	2362	1	C5H6N2	4-AMINOPYRIDINE 504-24-5
4	0.32		590		"	4-AMINOPYRIDINE
25	0.16		260		C5H6N2	4-METHYLPYRIMIDINE 3438-46-8
6	-0.72		2069		C5H6N2	PENTANEDINITRILE 544-13-8
7	-0.35		2412		C5H6N2	PYRIDAZINE,3-METHYL 1632-78-4
8	-0.32		2412		C5H6N2	PYRIDAZINE,4-METHYL 1120-88-3
9	-0.05		2412		C5H6N2	PYRIMIDINE,2-METHYL
830	0.01		2412		C5H6N2	PYRIMIDINE,5-METHYL 2036-41-1
1	-0.34		579		C5H6N2O1	1-ACETYLMIDAZOLE 2468-76-4
2	-0.87	2.0	447		C5H6N2O1	2-AMINOPYRIDINE-N-OXIDE 14150-95-9
3	-0.87	5.0	447	1	"	2-AMINOPYRIDINE-N-OXIDE
4	-0.87	7.4	447	1	"	2-AMINOPYRIDINE-N-OXIDE
35	-1.45		594		C5H6N2O1	2-PYRIMIDONE,4-METHYL 15231-48-8
6	-1.45		594		C5H6N2O1	2-PYRIMIDONE,6-METHYL
7	0.73		2412		C5H6N2O1	PYRAZINE,2-METHOXY 3149-28-8
8	0.08		2412		C5H6N2O1	PYRIDAZINE,3-METHOXY 19064-85-4
9	-0.31		2412		C5H6N2O1	PYRIDAZINE,4-METHOXY 20733-11-3
840	-1.32	7.4	2362	1	C5H6N2O1	PYRIDINE-3-HYDROXY-4-AMINO
1	0.23		2412		C5H6N2O1	PYRIMIDINE,2-METHOXY
2	0.54		2412		C5H6N2O1	PYRIMIDINE,4-METHOXY 6104-41-2
3	0.07		2412		C5H6N2O1	PYRIMIDINE,5-METHOXY
4	0.22		536	815	C5H6N2O1S1	4-HYDROXY-2-METHYLTHIO-PYRIMIDINE 20651-23-4
45	0.76		594		C5H6N2O1S1	THIAZOLE,2-ACETAMIDO 2719-23-5
8	-1.20		534		C5H6N2O2	1-METHYLURACIL 615-77-0
7	-0.77	7.4	594	1	C5H6N2O2	2,4-PYRIMIDINEDIONE,6-METHYL 626-48-2
8	-0.30		1375		C5H6N2O2	PYRIDAZINE,3,4-DIHYDROXY-6-METHYL
9	-0.62		536		C5H6N2O2	THYMINE 65-71-4
850	-0.49		1519	400	C5H6N2O2S1	3-SULFONAMIDOPYRIDINE 2438-76-8
1	0.94		2166		C5H6N2O3	1,2,5-OXADIAZOLE,3-METHYL-4-METHOXYCARBONYL
2	-1.94		547		C5H6N2O3	5-HYDROXYMETHYL-D2-URACIL 52565-39-6
3	-0.85	0.7	962		C5H6N2O3	BARBITURIC ACID,N-METHYL 2565-47-1
4	0.80		2166		C5H6N2O3	FURAZAN-2-OXIDE,3-METHYL-4-ACETYL

	logP	pH	Ref.	Note	MF	Name / CAS / activity
55	★	0.98	2166		C5H6N2O3	FURAZAN-2-OXIDE, 4-METHYL-3-ACETYL
6	★	0.56	2168		C5H6N2O4	FURAZAN-2-OXIDE, 3-METHYL-4-METHOXYCARBONYL
7	★	1.17	2412		C5H6N2S1	PYRAZINE, 2-METHYLTHIO 21948-70-9
8	★	1.01	2412		C5H6N2S1	PYRIMIDINE, 2-METHYLTHIO 823-09-6
9	★	-1.22	1404		C5H8N4O3	2(2-NO2-1-IMIDAZOLYL)ACETAMIDE
860	★	0.29	7.4	2206	306 C5H6N4O3	2-IMIDAZOLECARBOXAMIDE, 1-METHYL-5-NITRO
1	★	-0.43	7.4	2561	1 C5H8N4O3	2-NITROIMIDAZOLE-1-ACETALDOXIME
2	★	-0.38	1.0	2196	C5H6N4O3	PYRAZOLE, 3-METHYL-4-NITRO-5-CARBOXAMIDE
3	★	-0.38	7.4	2273	1 C5H6N4O4	1-TRIAZOLEACETIC ACID-3-NITRO, METHYL ESTER 70965-23-0
4	★	0.49	2387		C5H6N4O4	IMIDAZOLE, 1,2-DIMETHYL-4,5-DINITRO 19183-17-6
65	★	1.85	1478		C5H6O1	2-METHYLFURAN 534-22-5
6	★	0.87	1478		C5H8O1S1	2-HYDROXYMETHYLTHIOPHENE 636-72-6
7	★	1.44	1478		C5H6O2	2-METHOXYFURAN 25414-22-6
8	★	0.30	1478		C5H6O2	3-HYDROXYMETHYLFURAN 4412-91-3
9	★	0.22	7.0	2505	1 C5H6O2	FURFURYL ALCOHOL 98-00-0
870	★	0.28	1478		-	FURFURYL ALCOHOL
1	★	0.38	1825		C5H6O2S2	THIOPHENE, 2-MESYL 38695-58-8
2	★	2.33	1478		C5H8S1	2-METHYLTHIOPHENE 554-14-3
3	★	2.34	1478		C5H6S1	3-METHYLTHIOPHENE 616-44-4
4	★	0.05	7.4	2273	1 C5H7ClN4O3	1,2,4-TRIAZOLE, 3-NITRO-1-(3-CHLORO-2-HYDROXY)PROPYL 104958-94-3
75	★	-0.59	7.4	2361	1 C5H7F1N4O3	TRIAZOLE, 3-NITRO-1-(3-FLUORO-2-HYDROXY)PROPYL
6	★	-0.80	7.4	2361	1 C5H7F1N4O3	TRIAZOLE, 3-NITRO-1-(3-HYDROXY-2-FLUORO)PROPYL
7	★	1.21	570		C5H7N1	N-METHYLPYRROLE 96-54-8
8	★	0.37	1478		C5H7N1O1	2-AMINOMETHYLFURAN 617-89-0
9	★	-0.95	594		C5H7N1O2	N-METHYLSUCCINIMIDE 1121-07-0
880	★	-1.80	7.2	2323	468 C5H7N1O2	PROPARGYLGLYCINE
1	★	-0.25	7.4	401	1 C5H7N3	2,3-DIHYDRO-1H-IMIDAZO-PYRAZOLE 6714-29-0 antineoplastic
2	★	0.19	1519		C5H7N3	6-METHYL-4-PYRIMIDINAMINE 3435-28-7
3	★	0.35	2499		C5H7N3	PYRAZINE, 2-AMINO-6-METHYL
4	★	0.56	2444		C5H7N3	PYRAZINE, 2-METHYLAMINO 32111-28-7
85	★	-1.44	7.4	2362	1 C5H7N3	PYRIDINE, 3,4-DIAMINO 54-96-6
6	★	-0.85	1375		C5H7N3O1	3-AMINO-4-HYDROXY-6-METHYLPYRIDAZINE
7	★	-0.38	547		C5H7N3O1	4-ACETYLAMINOPYRAZOLE
8	★	0.63	2499		C5H7N3O1	PYRAZINE, 2-AMINO-5-METHOXY
9	★	0.73	2499		C5H7N3O1	PYRAZINE, 2-AMINO-6-METHOXY
890	★	0.56	2166		C5H7N3O2	1,2,5-OXADIAZOLE, 3-METHYL-4-(N-METHYL CARBOXAMIDO)
1	★	0.17	2166		C5H7N3O2	1,2,5-OXADIAZOLE, 3-METHYL-4-ACETYLAMINO
2	★	0.22	505		C5H7N3O2	5-ETHYL-6-AZAUACIL 19213-65-1
3	★	0.14	2387		C5H7N3O2	DIMETRIDAZOLE 551-92-8 antiprotozoal (vet)
4	★	0.30	7.4	2206	306	DIMETRIDAZOLE
95	★	0.64	7.4	2380	1	DIMETRIDAZOLE
6	★	-0.24	2387		C5H7N3O2	IMIDAZOLE, 1,2-DIMETHYL-4-NITRO 13230-04-1
7	★	-0.29	7.4	2206	306 C5H7N3O2	IMIDAZOLE, 1,5-DIMETHYL-4-NITRO 7464-88-8
8	★	-0.11	2387		C5H7N3O2	IMIDAZOLE, 1,5-DIMETHYL-4-NITRO
9	★	0.43	7.4	2206	306 C5H7N3O2	IMIDAZOLE, 2,4-DIMETHYL-5-NITRO
900	★	0.94	7.4	2206	306 C5H7N3O2S1	IMIDAZOL, 1-METHYL-2-METHYLTHIO-5-NITRO 1615-41-4
1	★	0.42	2166		C5H7N3O3	1,2,5-OXADIAZOLE, 3-METHYL-4-METHOXYCARBOXAMINO
2	★	-0.47	1003		C5H7N3O3	1-(2-HYDROXYETHYL)-2-NITROIMIDAZOLE 5008-67-7
3	★	-0.35	7.4	1022	1 C5H7N3O3	1-METHYL-2-NITRO-5-HYDROXYMETHYLIMIDAZOLE
4	★	-0.03	9.0	1409	C5H7N3O3	5-NITROIMIDAZOLE, 1-ME-2-HYDROXYMETHYL 936-05-0
5	★	0.19	2387		C5H7N3O3	IMIDAZOLE, 1-METHYL-4-NITRO-5-METHOXY 85012-71-1
6	★	0.21	2387		C5H7N3O3	IMIDAZOLE, 2-METHYL-4-NITRO-5-METHOXY 35687-42-4
7	★	0.13	1375		C5H7N3S1	3-AMINO-4-SULFHYDRYL-8-METHYLPYRIDAZINE
8	★	2.40	7.4	2648	448 C5H8	1,3-PENTADIENE, CIS
9	★	2.44	7.4	2648	448 C5H8	1,3-PENTADIENE, TRANS
910	★	2.48	547	60	C5H8	1,4-PENTADIENE 591-93-5
1	★	1.98	503		C5H8	1-PENTYNE 627-19-0
2	★	1.23	871		C5H8Br2N2O1	3,4-DIBROMO-N-NITROSOPIPERIDINE 57541-73-8
3	★	1.15	2550	459	C5H8Cl1N5	DESISOPROPYLATRAZINE
4	★	1.04	871		C5H8Cl2N2O1	3,4-DICHLORO-N-NITROSOPIPERIDINE 57541-72-7
15	★	1.84	591		C5H8Cl3N1O3	CARBOCLORAL 541-79-7 hypnotic
6	✓	0.75	2366	122	C5H8Cu1N6S2	COPPER(II)PYRUVALDEHYDE BIS(THIOSEMICARBAZONE)
7	★	0.47	594	400	C5H8N2	ACRYLONITRILE, 3-DIMETHYLAMINO
8	★	1.01	594		C5H8N2	PYRAZOLE, 3,5-DIMETHYL 67-51-6
9	★	0.80	547		C5H8N2O1	4-ETHOXYPYRAZOLE
920	★	1.18	871		C5H8N2O1	DELTA-3-N-NITROSOPIPERIDINE
1	★	1.18	2166		C5H8N2O1	FURAZAN, METHYLETHYL 17647-69-7
2	★	-0.48	7.0	1405	1 C5H8N2O2	HYDANTOIN, 5,5-DIMETHYL 77-71-4
3	★	-0.47	871		C5H8N2O2	N-NITROSO-4-PIPERIDONE 55556-91-7
4	★	-1.05	1728		C5H8N2O2	N-NITROSOPIPERIDONE
25	★	0.51	2188		C5H8N2O2S2	METHYLCARBAMIC ACID, 4-OXIMINO-1,3-DITHIOLANE ESTER
8	★	-0.68	505		C5H8N2O3	UREA, 1,3-DIACETYL 838-20-0
7	★	0.92	2166		C5H8N2O3S1	1,2,5-OXADIAZOLE, 3-METHYL-4-ETHYLSULFONYL
8	★	0.06	2188		C5H8N2O3S1	METHYLCARBAMIC ACID, 4-OXIMINO-1,3-OXATHIOLANE ESTER
9	★	0.65	2166		C5H8N2O4S1	FURAZAN-2-OXIDE, 3-METHYL-4-ETHYLSULFONYL
930	★	0.62	1519		C5H8N4	4-HYDRAZINO-6-METHYLPYRIMIDINE
1	★	-0.16	57		C5H8N4O1S1	3-METHIO-4-AMINO-8-ME-1,2,4-TRIAZINE-5-ONE 18826-96-5
2	★	0.30	2592		C5H8N4O2	1,2,4-TRIAZOLE, 1-PROPYL-3-NITRO
3	★	0.30	2166		C5H8N4O2	1,2,5-OXADIAZOLE, 3-(N'-METHYLUREIDO)-4-METHYL
4	★	-1.10	2387		C5H8N4O2	IMIDAZOLE, 1,2-DIMETHYL-4-NITRO-5-AMINO
35	★	-0.87	7.4	830	1 C5H8N4O2	N-DIAZOACETYLGLYCINE-N'-METHYLAMIDE
6	★	0.32	7.2	2036	1 C5H8N4O3S2	ACETAZOLAMIDE, N-METHYL 68300-47-0
7	★	0.49	7.2	2036	2	ACETAZOLAMIDE, N-METHYL
8	★	0.13	264		C5H8N4O3S2	METHAZOLAMIDE 554-67-4 diuretic, carbonic anhydrase inhibitor
9	★	1.24	1705		C5H8N4S1	GUANDINE, N2-(5-METHYLTHIAZOL-2-YL)

	logP	pH	Ref.	Note	MF	Name / CAS / activity	
940	★	1.27	595		C5H8N4S1	THIAZOLE,2-(3,3-DIMETHYL)TRIAZENYL	
1	★	1.24	1120		C5H8O1	2-ETHYLPROPENAL 922-63-4	
2	★	0.28	579		C5H8O1	2-METHYL-3-BUTYN-2-OL 115-19-5	
3	★	0.52	599		C5H8O1	3-PENTEN-2-ONE 625-33-2	
4	★	0.49	579		C5H8O1	CYCLOPROPYLMETHYL KETONE 765-43-5	
45	★	0.89	594	298	C5H8O1	PYRAN,2,3-DIHYDRO 110-87-2	
6	★	0.40	579		C5H8O2	ACETYLACETONE 123-54-6	
7	★	1.32	579		C5H8O2	ACRYLIC ACID,ETHYL ESTER 140-88-5	
8	★	0.97	594	400	C5H8O2	ALLYLACETATE 591-87-7	
9	★	-0.35	547		C5H8O2	D-VALEROLACTONE 542-28-9	
950	★	1.38	1402		C5H8O2	METHACRYLIC ACID,METHYL ESTER 80-62-6	
1	★	-0.21	1402		C5H8O3	ACRYLIC ACID,2-HYDROXYETHYL ESTER 818-61-1	
2	★	-2.18	594	1	C5H8O3	LEVULINIC ACID 123-76-2	
3	★	-0.49	570		"	LEVULINIC ACID	
4	★	0.39	594	342	C5H8O4	DIMETHYLMALONIC ACID 595-46-0	
55	★	-0.29	570		C5H8O4	GLUTARIC ACID 110-94-1	
6	★	-0.05	579		C5H8O4	MALONIC ACID,DIMETHYL ESTER 108-59-8	
7	★	1.24	1968	459	C5H9Au1Cl1N1	T-BUTYLISOCYANIDE GOLD CHLORIDE †	
8	★	0.86	401		C5H9Cl1F1N3O2	NITROUSUREA,3-(2-CHLOROETHYL)-1-(2-FLUOROETHYL) 13908-92-4	
9	★	1.53	401		C5H9Cl2N3O2	1,3-BIS(2-CHLOROETHYL)-1-NITROUSUREA 154-93-8 antineoplastic	
960	★	1.39	1942		C5H9F3O1	4,4,4-TRIFLUORO-2-METHYLBUTANOL	
1	★	1.37	1942		C5H9F3O1	4,4,4-TRIFLUORO-3-METHYLBUTANOL	
2	★	1.15	1942		C5H9F3O1	5,5,5-TRIFLUOROPENTANOL	
3	★	1.87	599		C5H9N1	1-PYRROLINE,2-METHYL	
4	★	1.10	579	400	C5H9N1	2-METHYLBUTYRONITRILE 18936-17-9	
65	★	1.07	1.0	579	400	C5H9N1	I-VALERONITRILE 625-28-5
6	★	0.98	7.0	579		C5H9N1	TRIMETHYLACETONITRILE 630-18-2
7	★	1.08	1.0	579	400	"	TRIMETHYLACETONITRILE
8	★	1.12	7.0	579	400	C5H9N1	VALERONITRILE 110-59-8
9	★	-0.46	579		C5H9N1O1	D-VALEROLACTAM 875-20-7	
970	★	-0.54	599		C5H9N1O1	N-METHYL-2-PYRROLIDINONE 872-50-4	
1	★	-0.32	594		C5H9N1O1	PYRROLIDINE,N-FORMYL 3760-54-1	
2	★	-2.54	7.0	1207	1	C5H9N1O2	PROLINE 147-85-3 amino acid
3	★	-2.50	7.0	2187	"	"	PROLINE
4	★	-3.17	1590	459	C5H9N1O3	HYDROXYPROLINE 51-35-4	
75	★	-4.19	1590	459	C5H9N1O4	GLUTAMIC ACID, MONOSODIUM SALT	
6	✓	-3.89	7.0	1207	1	C5H9N1O4	GLUTAMIC ACID 58-96-0 acidifier (gastric)
7	★	-0.22	2114		"	"	GLUTAMIC ACID
8	★	0.13	561		C5H9N1S1	2-AZACYCLOHEXANTHIONE 13070-01-4	
9	★	2.82	1947		C5H9N1S1	2-METHYLPROPANE,ISOTHIOCYANATO 591-82-2	
980	★	2.81	1947		C5H9N1S1	BUTANE,2-ISOTHIOCYANATO	
1	★	2.92	1947		C5H9N1S1	BUTANE,ISOTHIOCYANATO 592-82-5	
2	★	2.03	502		C5H9N1S1	THIOCYANIC ACID,BUTYL ESTER 628-83-1	
3	★	-0.70	1853		C5H9N3	HISTAMINE 51-45-6 stimulant (gastric)	
4	★	0.20	1137		C5H9N3O1	2-AMINO-5-I-PROPYL-1,3,4-OXADIAZOLE	
85	★	0.23	1137		C5H9N3O1	2-AMINO-5-PROPYL-1,3,4-OXADIAZOLE	
8	★	1.40	2097		C5H9N3O1	DIAZINECARBONITRILE,T-BUTYL,OXIDE	
7	★	-0.49	723		C5H9N5O1	2,4-DIAMINO-6-METHYLAMINO-PYRIMIDINE-3-OXIDE	
8	★	3.00	547	400	C5H10	CYCLOPENTANE 287-82-3	
9	★	0.30	977		C5H10Cl1N3O3	HYDROXYETHYL-CNU 60784-46-5 antineoplastic	
990	★	0.36	1728		C5H10N2O1	N-NITROSOPIPERIDINE 100-75-4	
1	★	-0.03	1728		C5H10N2O2	2-METHYL-N-NITROSOMORPHOLINE	
2	★	0.04	673		C5H10N2O2	2-METHYLPROPANOYLUREA	
3	★	-0.47	871		C5H10N2O2	3-HYDROXY-N-NITROSOPIPERIDINE	
4	★	-0.89	871		C5H10N2O2	4-HYDROXY-N-NITROSOPIPERIDINE	
95	★	-0.13	1624		C5H10N2O2	ACETONE,O-((MEAMINO)CARBONYL)OXIME 10520-34-0	
6	★	-1.52	1591		C5H10N2O2	ALANIN-AMIDE,N-ACETYL	
7	★	-1.41	7.0	2309	1	"	ALANIN-AMIDE,N-ACETYL
8	★	-0.01	2198		C5H10N2O2	ETHYLUREA,N'-ACETYL	
9	★	-1.56	1558		C5H10N2O2	GLYCINE,N-ACETYL-N'-METHYLAMINO-AMIDE	
1000	★	-0.29	7.1	1591	C5H10N2O2S1	CYSTEIN-AMIDE,N-ACETYL	
1	★	0.60	1629		C5H10N2O2S1	METHOMYL 16752-77-5 insecticide-nematocide	
2	★	-3.15	1590	459	C5H10N2O3	GLUTAMINE 56-85-9	
3	★	-1.87	1591		C5H10N2O3	SERIN-AMIDE,N-ACETYL	
4	★	-0.28	871		C5H10N4O2	2-METHYL,N,N'-DINITROSOPIPERAZINE 55556-94-0	
5	★	-0.25	1728		C5H10N4O2	2-METHYL,N,N'-DINITROSOPIPERAZINE	
6	★	-0.51	871		C5H10N4O2	N,N'-DINITROSOHOMOPIPERAZINE 55557-00-1	
7	★	-0.30	4.0	979	364	C5H10N6O4	1,1'-PROPYLEN-BIS(1-NITROUSUREA) 27640-19-3
8	★	0.84	594	400	C5H10O1	2-BUTANONE,3-METHYL 563-80-4	
9	★	0.91	566	1	C5H10O1	2-PENTANONE 107-87-9	
1010	★	0.99	1560	100	C5H10O1	3-PENTANONE 98-22-0	
1	★	0.85	579		C5H10O1	TETRAHYDROPYRAN 142-68-7	
2	★	0.46	579	400	C5H10O2	2,2-DIMETHYL-1,3-DIOXOLANE 2916-31-6	
3	★	1.18	579	400	C5H10O2	2-METHYLBUTYRIC ACID 116-53-0	
4	★	1.24	1560	100	C5H10O2	ACETIC ACID,PROPYL ESTER 109-60-4	
15	★	1.47	1.0	579	C5H10O2	ACETIC ACID,TRIMETHYL 75-98-9	
6	★	-0.10	2562		C5H10O2	ENTYLENE GLYCOL,MONOALLYL ETHER 111-45-5	
7	★	0.36	2596		C5H10O2	ETHYL GLYCIDYL ETHER 4016-11-9	
8	★	1.16	1.0	579	400	C5H10O2	I-VALERIC ACID 503-74-2
9	★	1.29	594	400	C5H10O2	METHYLBUTYRATE 623-42-7 flavoring (artificial rum & fruit essences)	
1020	★	1.21	503		C5H10O2	PROPIONIC ACID,ETHYL ESTER 105-37-3	
1	★	1.39	1135	537	C5H10O2	VALERIC ACID 109-52-4	
2	★	1.21	579		C5H10O3	DIETHYLCARBONATE 105-58-8	
3	★	-0.06	1266		C5H10O3	METHYL-4-HYDROXYBUTYRATE 925-57-5	
4	★	-3.02	1087		C5H10O5	ARABINOSE 147-81-9	

logP	pH	Ref.	Note	MF	Name / CAS / activity
25 ★	-2.32	7.4	293	1 C5H10O5	RIBOSE 50-69-1
6 ★	3.37		1560	100 C5H11Br1	1-BROMOPENTANE 110-53-2
7 ★	2.52		594	400 C5H11Cl1	BUTANE,2-CHLORO-2-METHYL 594-36-5
8 ★	2.33		503	C5H11F1	1-FLUOROPENTANE 592-50-7
9 ★	0.81	13.0	568	224 C5H11N1	ALLYLETHYLAMINE 2424-02-4
1030 ★	0.92	12.0	594	400 C5H11N1	N-METHYLPYRROLIDINE 120-94-5
1 ★	0.64	13.0	588	224 C5H11N1	PIPERIDINE 110-89-4
2 ★	-0.11		594	C5H11N1O1	DIMETHYLPROPIONAMIDE 758-96-3
3 ★	-0.33		505	C5H11N1O1	MORPHOLINE,N-METHYL 109-02-4
4 ★	2.01		547	400 C5H11N1O2	1-NITROPENTANE 628-05-7
35 ★	-2.63		2018	C5H11N1O2	5-AMINOPENTANOIC ACID 660-88-8
6 ★	-2.11		2654	448 C5H11N1O2	A-AMINOVALERIC ACID 6600-40-4
7 ★	-1.93	7.2	2323	468 "	A-AMINOVALERIC ACID
8 ★	0.89		594	400 C5H11N1O2	N,N-DIMETHYLETHYL CARBAMATE 687-48-9
9 ★	0.85	7.4	172	1 C5H11N1O2	O-BUTYL CARBAMATE 592-35-8
1040 ★	0.65	7.4	172	1 C5H11N1O2	O-I-BUTYL CARBAMATE 543-28-2
1 ★	0.95		702	C5H11N1O2	O-PROPYL-N-METHYL CARBAMATE 17671-76-0
2 ★	0.48	7.4	172	1 C5H11N1O2	O-T-BUTYL CARBAMATE 4248-19-5
3 ★	-2.26	7.0	1207	1 C5H11N1O2	VALINE 72-18-4 amino acid
4 ★	-2.08	7.0	2197	"	VALINE
45 ★	-1.87		405	C5H11N1O2S1	METHIONINE 63-68-3 amino acid
6 ★	-1.78		1590	459 C5H11N1O2S1	PENICILLAMINE 52-67-5 chelating agent
7 ★	-2.51	7.2	2323	468 C5H11N1O3	ETHYLSERINE
8 ★	2.84		579	C5H11N1O3	ISOAMYL NITRATE 543-87-3
9 ★	-3.10	7.2	2323	468 C5H11N1O4S1	METHIONINESULFONE
1050 ★	0.20		871	C5H11N3O1	4-METHYL-N-NITROSOPIPERAZINE 16339-07-4
1 ★	1.04	4.0	979	364 C5H11N3O2	1-(I-BUTYL)-1-NITROSOUREA 760-60-1
2 ★	1.04	4.0	979	364 C5H11N3O2	1-BUTYL-1-NITROSOUREA 869-01-2
3 ★	0.71		671	C5H11N3O2	1-NITROSO-1-ETHYL-3,3-DIMETHYLUREA 50285-71-7
4 ★	0.86		579	C5H11O4P1	PHOSPHONIC ACID,2-OXOPROPYL,DIMETHYL ESTER 4202-14-6
55 ★	3.11		547	400 C5H12	NEOPENTANE 463-82-1
6 ★	3.39		547	822 C5H12	PENTANE 109-66-0
7 ★	0.78		1693	C5H12N1O3P1S2	DIMETHOATE 60-51-5 insecticide
8 ★	-0.28	9.0	547	400 C5H12N2	N-AMINOPIPERIDINE 2213-43-6
9 ★	-0.35		1137	C5H12N2O1	2,2-DIMETHYLPROPIONIC ACID HYDRAZIDE 17883-59-9
1060 ★	-0.33		1137	C5H12N2O1	2-METHYLBUTYRIC ACID HYDRAZIDE
1 ★	-0.31		1137	C5H12N2O1	I-VALERIC ACID HYDRAZIDE 24310-18-7
2 ★	1.02		2570	C5H12N2O1	METHYLBUTYLNITROSAMINE 7068-83-9
3 ★	0.41		547	C5H12N2O1	N-BUTYLUREA 592-31-4
4 ★	0.90		2570	C5H12N2O1	N-NITROSOETHYL-I-PROPYL AMINE 16339-04-1
65 ★	0.76		2570	C5H12N2O1	N-NITROSOMETHYL-T-BUTYL AMINE 2504-18-9
6 ★	0.19		579	C5H12N2O1	TETRAMETHYLUREA 632-22-4
7 ★	-0.11		1137	C5H12N2O1	VALERIC ACID HYDRAZIDE 38291-82-6
8 ★	0.32	7.4	1184	1 C5H12N2O2	3-BUTYLHYDROXYUREA 5681-57-2
9 ★	-4.41	7.2	2323	468 C5H12N2O2	ORNITHINE 70-26-8 anticholestemic
1070 ★	0.57	6.5	2013	C5H12N2S1	THIOUREA,N,N'-DIETHYL 105-55-5
1 ★	0.49	6.5	2013	C5H12N2S1	THIOUREA,TETRAMETHYL 2782-81-4
2 ★	-1.28	10.1	401	1 C5H12N8	MITOGUAZONE 7059-23-6 antineoplastic +
3 ★	1.31		2126	C5H12O1	1-PROPANOL,2,2-DIMETHYL 75-84-3
4 ★	1.19		2126	C5H12O1	2-PENTANOL 6032-29-7
75 ★	0.89		504	C5H12O1	2-PROPANOL,2-ETHYL 75-85-4 solvent
6 ★	1.28		425	C5H12O1	3-METHYL-2-BUTANOL 598-75-4
7 ★	1.21		547	400 C5H12O1	3-PENTANOL 584-02-1
8 ★	1.66		594	400 C5H12O1	BUTYL METHYLETHYR 828-28-4
9 ★	1.16		2126	C5H12O1	I-PENTANOL 123-51-3
1080 ★	0.94		1952	C5H12O1	METHYL-T-BUTYLETHER 1634-04-4 cholelitholytic agent
1 ★	1.56		547	400 C5H12O1	PENTANOL 71-41-0
2 ★	0.84		505	C5H12O2	DIETHOXYMETHANE 462-95-3
3 ★	0.05		768	C5H12O2	I-PROPOXYETHANOL 109-59-1
4 ★	-0.09		594	400 C5H12O2	PROPANE,1,2-DIMETHOXY 7778-85-0
85 ★	-0.86	7.0	834	1 C5H13N1	AMYLAMINE 110-58-7
6 ★	1.49	13.0	588	224 "	AMYLAMINE
7 ★	0.93	13.0	588	224 C5H13N1	ETHYL-I-PROPYLAMINE 19961-27-4
8 ★	1.33		505	C5H13N1	METHYLBUTYLAMINE 110-68-9
9 ★	0.41	13.0	594	2 C5H13N3	TETRAMETHYLGUANIDINE 80-70-6
1090 ★	-0.62		1394	C5H13N3O1	4,4-DIETHYLSEMICARBAZIDE
1 ★	-0.60		1394	C5H13N3O1	4-BUTYLSEMICARBAZIDE 20605-19-0
2 ★	-0.84		1394	C5H13N3O1	4-ISOBUTYLSEMICARBAZIDE
3 ★	-0.81		1394	C5H13N3O1	4-T-BUTYLSEMICARBAZIDE
4 ★	0.71		2182	459 C5H13O2P1S1	METHYLPHOSPHONIC ACID,O-ETHYL,S-ETHYL ESTER 2511-10-6
95 ★	2.08		2182	459 C5H13O2P1S1	METHYLTHIOPHOSPHONIC ACID,DIETHYL ESTER 6998-81-2
6 ★	3.22		512	C5H13Si1	SILANE,DIMETHYL-PROPYL 18143-31-2
7 ★	-3.71		549	466 C5H14N1O1.Br1	CHOLINEBROMIDE 1927-06-6
8 ★	0.65		600	C5H14N1O2P1S1	O,S-DIMETHYL-N-PROPYL-PHOSPHORAMIDOTHIOATE 16271-16-2
9 ★	-3.00		524	820 C5H14N1.I1	TRIMETHYL-ETHYL-AMMONIUM IODIDE 61-93-4
1100 ★	-0.20	13.0	594	400 C5H14N2	N,N,N'-TRIMETHYLETHYLENEDIAMINE 142-25-6
1 ★	-0.67		1908	C5H15N2O1P1	PHOSPHONICDIAMIDE,PENTAMETHYL 2511-17-3
2 ★	6.07		1814	459 C6Br6	HEXABROMOBENZENE 87-82-1
3 ★	4.22		1364	C6Cl5N1O2	PENTACHLORONITROBENZENE 82-68-8 fungicide (soil)
4 ★	5.73		2293	400 C6Cl6	HEXACHLOROBENZENE 118-74-1 fungicide
5 ★	2.55		594	400 C6F6	HEXAFLUOROBENZENE 392-56-3
6 ★	2.91		579	C6F12	CYCLOHEXANE,PERFLUORO 355-68-0
7 ★	0.95		2499	C6H1Cl1N4	PYRAZINE,2,3-DICYANO-5-CHLORO
8 ★	3.89		1710	C6H1Cl4N1O2	2,3,5,6-TETRACHLORONITROBENZENE 117-18-0
9 ★	4.17	7.3	509	2 C6H1Cl4N3	4,5,6,7-TETRACHLOROBENZOTRIAZOLE 2338-10-5

	logP	pH	Ref.	Note	MF	Name / CAS / activity
1110	★ 5.18		2293	400	C6H1Cl5	PENTACHLOROBENZENE 608-93-5
1	★ 5.12	1.4	536	342	C6H1Cl5O1	PENTACHLOROPHENOL 87-86-5 <i>herbicide--preservative(wood)</i>
2	★ 2.53		594		C6H1F5	PENTAFLUOROBENZENE 383-72-4
3	★ 3.23		359	824	C6H1F5O1	PENTAFLUOROPHENOL 771-61-9
4	★ 5.13		1600		C6H2Br4	1,2,4,5-TETRABROMOBENZENE 636-28-2
15	★ 3.81		1710		C6H2Cl3N1O2	2,3,4-TRICHLORONITROBENZENE 17700-09-3
6	★ 3.48		1710		C6H2Cl3N1O2	2,4,5-TRICHLORONITROBENZENE 89-69-0
7	★ 3.93		2134		C6H2Cl3N1O3	PHENOL,2,3,6-TRICHLORO-4-NITRO 20404-02-8
8	★ 4.64		2293	400	C6H2Cl4	1,2,3,4-TETRACHLOROBENZENE 634-66-2
9	★ 4.66		2293	400	C6H2Cl4	1,2,3,5-TETRACHLOROBENZENE 634-90-2
1120	★ 4.80		2293	400	C6H2Cl4	1,2,4,5-TETRACHLOROBENZENE 95-94-3
1	★ 4.21		1709		C6H2Cl4O1	2,3,4,5-TETRACHLOROPHENOL 4901-51-3
2	★ 4.45		1554		C6H2Cl4O1	2,3,4,6-TETRACHLOROPHENOL 58-90-2
3	★ 3.88		1709		C6H2Cl4O1	2,3,5,6-TETRACHLOROPHENOL 935-95-5
4	★ 4.29		1554		C6H2Cl4O2	TETRACHLORO-1,2-BENZENEDIOL 1198-55-6
25	★ 5.08		2293	400	C6H2Cl5N1	PENTACHLOROANILINE 627-20-8
6	✓ 0.13		567	820	C6H2N3O7.C4H12N1	TETRAMETHYL AMMONIUM PICRATE
7	✓ 1.01		1701	820	C6H2N3O7.C6H11F3N1	N,N,N-TRIME-2,2,2-TRIFLUOROETAMININE PICRATE
8	0.48		567	820	C6H2N3O7.C5H14N1	ETHYLTRIMETHYL AMMONIUM PICRATE
9	✓ 0.60		1701	820	"	ETHYLTRIMETHYL AMMONIUM PICRATE
1130	★ 0.38		2499		C6H2N4	PYRAZINE,2,3-DICYANO
1	3.25		1283		C6H3Br1Cl1N1O2	3-CHLORO-4-BROMONITROBENZENE 29682-39-1
2	★ 3.57		2134		C6H3Br2N1O3	2,6-DIBROMO-4-NITROPHENOL 99-28-5
3	★ 4.51		1600		C6H3Br3	1,3,5-TRIBROMOBENZENE 626-39-1
4	3.96		359	824	C6H3Br3O1	2,4,6-TRIBROMOPHENOL 118-79-6
35	4.13		1400	459	"	2,4,6-TRIBROMOPHENOL
6	4.23		757		"	2,4,6-TRIBROMOPHENOL
7	★ 4.37	1.4	536	342	C6H3Br3O2	2,4,6-TRIBROMORESORCINOL 2437-49-2
8	★ 2.18		2410		C6H3Cl1N2O4	1,2-DINITROBENZENE,4-CHLORO
9	2.17		2163	459	C6H3Cl1N2O4	BENZENE,1-CHLORO-2,4-DINITRO 97-00-7
1140	-1.30		1008	837	C6H3Cl1N2O6S1	2,4-DINITROBENZENESULFONYLCHLORIDE
1	★ 1.79		332		C6H3Cl1N2S1	THIENO(2,3-D)-PYRIMIDINE,4-CHLORO 16289-66-2
2	★ 0.84		599		C6H3Cl1O2	2-CHLOROBENZOQUINONE
3	★ 3.05		1710		C6H3Cl2N1O2	2,3-DICHLORONITROBENZENE 3209-22-1
4	★ 3.09		1710		C6H3Cl2N1O2	2,4-DICHLORONITROBENZENE 89-61-2
45	★ 3.12		1710		C6H3Cl2N1O2	3,4-DICHLORONITROBENZENE 99-54-7
6	★ 2.90		2305	459	C6H3Cl2N1O2	NITROBENZENE,2,5-DICHLORO
7	★ 3.13		2305	459	C6H3Cl2N1O2	NITROBENZENE,3,5-DICHLORO
8	★ 2.94		359	824	C6H3Cl2N1O3	2,6-DICHLORO-4-NITROPHENOL 618-90-4
9	★ 4.14		2293	400	C6H3Cl3	1,2,3-TRICHLOROBENZENE 87-61-6
1150	★ 4.02		2000		C6H3Cl3	1,2,4-TRICHLOROBENZENE 120-82-1
1	★ 4.19		2293	400	C6H3Cl3	1,3,5-TRICHLOROBENZENE 108-70-3
2	0.30		1178		C6H3Cl3N2O2	PICLORAM 1918-02-1 <i>herbicide</i>
3	★ 3.51		1400	459	C6H3Cl3O1	2,3,4-TRICHLOROPHENOL 15950-66-0
4	3.54		1505	459	"	2,3,4-TRICHLOROPHENOL
55	3.80		1709		"	2,3,4-TRICHLOROPHENOL
6	3.84		1709		C6H3Cl3O1	2,3,5-TRICHLOROPHENOL 933-78-8
7	4.56		1400	459	"	2,3,5-TRICHLOROPHENOL
8	★ 3.77		1709		C6H3Cl3O1	2,3,6-TRICHLOROPHENOL 933-75-5
9	★ 3.72		508		C6H3Cl3O1	2,4,5-TRICHLOROPHENOL 95-85-4 <i>fungicide</i>
1160	★ 3.69		508		C6H3Cl3O1	2,4,6-TRICHLOROPHENOL 88-06-2
1	★ 4.01		579		C6H3Cl3O1	3,4,5-TRICHLOROPHENOL 609-19-8
2	★ 4.26		1822	459	"	3,4,5-TRICHLOROPHENOL
3	★ 3.71		1738	459	C6H3Cl3O2	3,4,5-TRICHLOROCATECHOL 56961-20-7
4	3.60		1738	459	C6H3Cl3O2	3,4,6-TRICHLOROCATECHOL 32139-72-3
65	★ 4.04		1505	459	C6H3Cl4N1	2,3,4,5-TETRACHLOROANILINE 634-83-3
6	★ 4.57		2293	400	"	2,3,4,5-TETRACHLOROANILINE
7	★ 4.48		2293	400	C6H3Cl4N1	2,3,5,6-TETRACHLOROANILINE 3481-20-7
8	★ 3.41		1190		C6H3Cl4N1	NITRAPYRIN
9	★ 2.41		594	400	C6H3F3	1,2,4-TRIFLUOROBENZENE 367-23-7
1170	0.62		1412		C6H3F6N5O2	1,2,4-TRIAZOLE,3,5-DI(TRIFLUOROACETAMIDO)
1	1.68		848		C6H3I3O2	2,4,6-TRI-IODO-RESORCINOL
2	-2.46		1463		C6H3N2O6	2,4-DINITROPHENOLATEANION
3	★ 1.18		536		C6H3N3O6	1,3,5-TRINITROBENZENE 99-35-4
4	✓ 1.39		1701	820	C6H3N3O7	2,2,2-TRIFLUOROETHYLAMINE PICRATE
75	★ 0.89	1.0	579	342	C6H3N3O7	2,4,6-TRINITROPHENOL 88-89-1
6	✓ 2.05		567	820	C6H3N3O7	BUTYLAMINE PICRATE
7	✓ 1.29		567	820	C6H3N3O7	DIETHYLAMINE PICRATE
8	✓ 0.76		567	820	C6H3N3O7	DIMETHYLAMINE PICRATE
9	✓ 1.03		567	820	C6H3N3O7	ETHYLAMINE PICRATE
1180	✓ 1.89		587	820	C6H3N3O7	I-BUTYLAMINE PICRATE
1	✓ 1.37		587	820	C6H3N3O7	I-PROPYLAMINE PICRATE
2	✓ 0.70		576	820	C6H3N3O7	METHYLAMINE PICRATE
3	✓ 1.29		1701	820	C6H3N3O7	N,N-DIMETHYL-2,2,2-TRIFLUOROETHYLAMINE PICRATE
4	✓ 1.51		1701	820	C6H3N3O7	N-ETHYL-2,2,2-TRIFLUOROETHYLAMINE PICRATE
85	✓ 1.37		1701	820	C6H3N3O7	N-METHYL-2,2,2-TRIFLUOROETHYLAMINE PICRATE
6	✓ 1.50		567	820	C6H3N3O7	PROPYLAMINE PICRATE
7	✓ 1.80		567	820	C6H3N3O7	S-BUTYLAMINE PICRATE
8	✓ 1.68		567	820	C6H3N3O7	T-BUTYLAMINE PICRATE
9	✓ 0.60		567	820	C6H3N3O7	TRIMETHYLAMINE PICRATE
1190	-1.31	7.4	1966	1	C6H4Au1Cl2N1O2	1,1-DICHLORO-1,3,2-OXAZAURO(3,4)PYRIDIN-3-ONE +
1	★ 1.12		538		C6H4Br1N1O1	N-BROMOBENZOQUINONEMONIMINE
2	★ 2.64		501		C6H4Br1N1O2	BENZENE,3-BROMO-1-NITRO 585-79-5
3	2.98	7.0	925	1	C6H4Br1N1O2	BENZENE,4-BROMO-1-NITRO 588-78-7
4	★ 2.55		897		"	BENZENE,4-BROMO-1-NITRO

logP	pH	Ref.	Note	MF	Name / CAS / activity
95 ★	2.52	547		C8H4Br1N1O2	O-BROMONITROBENZENE 577-19-5
6 ★	2.45	1946		C8H4Br1N1O3	FURAN,2-(2-BROMOETHENYL)-5-NITRO 67363-72-6
7 ★	3.75	536		C8H4Br2	M-DIBROMOBENZENE 106-36-1
8 ★	3.64	536		C8H4Br2	O-DIBROMOBENZENE 583-53-9
9 ★	3.79	1600		C8H4Br2	P-DIBROMOBENZENE 106-37-6
1200 ★	3.22	359	824	C8H4Br2O1	2,4-DIBROMOPHENOL 615-58-7
1 ★	3.36	2645	225	C8H4Br2O1	2,6-DIBROMOPHENOL 608-33-3
2 ★	1.26	538		C8H4Cl1N1O1	N-CHLOROBENZOQUINONEMONIMINE 637-61-6
3 ★	-1.70	1190		C8H4Cl1N1O2	6-CHLOROPICOLINIC ACID 4684-64-0
4 ★	2.24	531		C8H4Cl1N1O2	BENZENE,2-CHLORO-1-NITRO 88-73-3
5 ★	2.46	501		C8H4Cl1N1O2	BENZENE,3-CHLORO-1-NITRO 121-73-3
6 ★	2.39	501		C8H4Cl1N1O2	BENZENE,4-CHLORO-1-NITRO 100-00-5
7 ★	0.73	7.4 1075	324	C8H4Cl1N1O3	2-CHLORO-4-NITROPHENOL 619-08-9
8 ★	2.46	1.5 2329	314	C8H4Cl1N1O3	PHENOL,2-NITRO-4-CHLORO 89-64-5
9 ★	3.53	2293	400	C8H4Cl2	1,3-DICHLOROBENZENE 541-73-1
1210 ★	3.43	2293	400	C8H4Cl2	O-DICHLOROBENZENE 95-50-1 herbicide-insecticide
1 ★	3.44	2293	400	C8H4Cl2	P-DICHLOROBENZENE 106-46-7 fumigant
2 ★	1.80	2506		C8H4Cl2N2O2	DICHLORAN 99-30-9 fungicide
3 ★	2.84	1505	459	C8H4Cl2O1	2,3-DICHLOROPHENOL 576-24-9
4 ★	3.06	359	824	C8H4Cl2O1	2,4-DICHLOROPHENOL 120-83-2
15 ★	3.06	1400	459	C8H4Cl2O1	2,5-DICHLOROPHENOL 583-78-8
6 ★	2.75	2215		C8H4Cl2O1	2,6-DICHLOROPHENOL 87-85-0
7 ★	3.33	1690	459	C8H4Cl2O1	3,4-DICHLOROPHENOL 95-77-2
8 ★	3.62	572		C8H4Cl2O1	3,5-DICHLOROPHENOL 591-35-5
9 ★	3.68	2293	400	C8H4Cl3N1	2,3,4-TRICHLOROANILINE 634-67-3
1220 ★	3.69	2293	400	C8H4Cl3N1	2,4,5-TRICHLOROANILINE 636-30-6
1 ★	3.69	2293	400	C8H4Cl3N1	2,4,6-TRICHLOROANILINE 634-93-5
2 ★	3.32	1505	459	C8H4Cl3N1	3,4,5-TRICHLOROANILINE 634-91-3
3 ★	4.27	1190		C8H4Cl3N1O1	2-METHOXY-3,5,6-TRICHLOROPYRIDINE 31557-34-3
4 ★	4.31	1140		C8H4Cl6	HEXACHLOROCYCLOHEXENE 57722-15-3
25 ★	4.34	1140		"	HEXACHLOROCYCLOHEXENE 57722-16-4
6 ★	4.35	1140		"	HEXACHLOROCYCLOHEXENE 57722-17-5
7 ★	4.12	1140		"	HEXACHLOROCYCLOHEXENE 59229-56-0
8 ★	1.90	7.0 925	1	C8H4F1O2	M-FLUORONITROBENZENE 402-67-5
9 ★	1.69	547		C8H4F1O2	O-FLUORONITROBENZENE 1493-27-2
1230 ★	1.80	7.0 925	1	C8H4F1O2	P-FLUORONITROBENZENE 350-46-9
1 ★	1.91	1.5 2329	314	C8H4F1O3	PHENOL,2-NITRO-5-FLUORO 446-36-6
2 ★	2.37	594	400	C8H4F2	BENZENE,1,2-DIFLUORO 367-11-3
3 ★	1.46	7.4 2648	448	C8H4F2O1	PHENOL,2,6-DIFLUORO 28177-48-2
4 ★	2.05	594	400	"	PHENOL,2,6-DIFLUORO
35 ★	1.54	1412		C8H4F7N5O1	1,2,4-TRIAZOLE,3-AMINO,5-HEPTAFLUOROBUTYRAMIDO
6 ★	2.84	562		C8H4I1O2	M-IODONITROBENZENE 645-00-1
7 ★	4.11	594	400	C8H4I2	BENZENE,1,4-DIODO 624-38-4
8 ★	0.40	594	400	C8H4N2	2-CYANOPYRIDINE 100-70-9
9 ★	-0.44	7.2 2317	1	C8H4N2	3-CYANOPYRIDINE 100-54-9
1240 ★	0.23	2412		"	3-CYANOPYRIDINE
1 ★	0.46	163	459	C8H4N2	4-CYANOPYRIDINE 100-48-1
2 ★	-0.94	1716		C8H4N2O1	4-CYANOPYRIDINEOXIDE 14906-59-3
3 ★	1.69	2166		C8H4N2O1	BENZOFURAZAN 273-09-6
4 ★	1.43	2166		C8H4N2O2	BENZOFURAZAN-2-OXIDE
45 ★	1.49	531		C8H4N2O4	M-DINITROBENZENE 99-65-0
6 ★	1.69	547		C8H4N2O4	O-DINITROBENZENE 528-29-0
7 ★	1.46	501		C8H4N2O4	P-DINITROBENZENE 100-25-4
8 ★	-0.39	1463		C8H4N2O5	2,4-DINITROPHENOLATE,POTASSIUM SALT
9 ★	1.67	1.5 2329	314	C8H4N2O5	2,4-DINITROPHENOL 51-28-5
1250 ★	1.75	503		C8H4N2O5	2,5-DINITROPHENOL 329-71-6
1 ★	1.37	1.0 572	342	C8H4N2O5	2,6-DINITROPHENOL 573-56-8
2 ★	2.36	505		C8H4N2O5	3,5-DINITROPHENOL 586-11-8
3 ★	1.30	1946		C8H4N2O5	FURAN,2-(2-NITROETHENYL)-5-NITRO
4 ★	2.10	995		C8H4N2O6	2,4-DINITRORESORCINOL 519-44-8
55 ★	2.01	590	60	C8H4N2S1	2,1,3-BENZOTHIADIAZOLE 273-13-2
6 ★	1.64	2166		C8H4N2Se1	2,1,3-BENZOSELENADIAZOLE 273-15-4
7 ✓	-0.13	505		C8H4N4	ISOPROPENYLAMINE,1,1,3-TRICYANO 868-54-2
8 ★	-0.58	1627		C8H4N4	PTERIDINE 91-18-9
9 ★	1.95	7.3 509	2	C8H4N4O2	5-NITROBENZOTRIAZOLE 2338-12-7
1260 ★	0.20	2649		C8H4O2	QUINONE 106-51-4
1 ★	2.99	501		C8H5Br1	BROMOBENZENE 108-96-1
2 ★	-2.50	7.4 2071		C8H5Br1Hg1O3S1	P-BROMOMERCURIPHENYLSULFONIC ACID +
3 ★	-0.88	1375		C8H5Br1N4O1	1,2,4-TRIAZOLO(4,3-B)PYRIDAZINE-6-ME-7-BR-8-OH
4 ★	2.63	501		C8H5Br1O1	M-BROMOPHENOL 591-20-8
65 ★	2.35	501		C8H5Br1O1	O-BROMOPHENOL 95-56-7
6 ★	2.59	501		C8H5Br1O1	P-BROMOPHENOL 106-41-2
7 ★	1.84	2523		C8H5Br1O3	FURAN,2-BROMO-5-METHOXYCARBONYL
8 ★	2.89	594	400	C8H5Cl1	CHLOROBENZENE 108-90-7
9 ★	2.06	1772		C8H5Cl1F1N1	3-CHLORO-4-FLUOROANILINE 367-21-5
1270 ★	1.78	594		C8H5Cl1Hg1	PHENYLMERCURIC CHLORIDE 100-56-1 antimicrobial-fungicide
1 ★	1.51	1135	537	C8H5Cl1Hg1O1	CHLOROMERCURIPHENOL 90-03-9 disinfectant
2 ★	2.72	2159		C8H5Cl1N2O2	2-NITRO-4-CHLOROANILINE 89-63-4
3 ★	2.06	594		C8H5Cl1N2O2	ANILINE,4-CHLORO-3-NITRO 835-22-3
4 ★	0.47	2642		C8H5Cl1N2O2	PYRAZINE,2-CHLORO-6-METHOXYCARBONYL
75 ★	0.47	2499		C8H5Cl1N2O2	PYRAZINE,2-CHLORO-6-METHOXYCARBONYL
6 ★	1.53	1549		C8H5Cl1N2O3	2-AMINO-6-CHLORO-4-NITROPHENOL 6358-08-4
7 ★	2.50	501		C8H5Cl1O1	M-CHLOROPHENOL 108-43-0
8 ★	2.15	501		C8H5Cl1O1	O-CHLOROPHENOL 96-67-8
9 ★	2.39	501		C8H5Cl1O1	PARACHLORPHENOL 108-48-9 antibacterial (topical)



logP	pH	Ref.	Note	MF	Name / CAS / activity
1280	1.80	1568		C6H5ClO2	4-CHLORORESORCINOL 95-88-5
1 *	1.40	1153		C6H5ClO2	CHLOROHYDROQUINONE 615-67-8
2 *	2.86	2293	400	C6H5Cl2N1	2,3-DICHLOROANILINE 608-27-5
3 *	2.91	2293	400	C6H5Cl2N1	2,4-DICHLOROANILINE 554-00-7
4 *	2.92	2293	400	C6H5Cl2N1	2,5-DICHLOROANILINE 95-82-9
85 *	2.82	2293	400	C6H5Cl2N1	2,6-DICHLOROANILINE 608-31-1
6 *	2.69	530		C6H5Cl2N1	3,4-DICHLOROANILINE 95-76-1
7 *	2.90	1505	459	C6H5Cl2N1	3,5-DICHLOROANILINE 626-43-7
8	1.44	264		C6H5Cl2N1O2S1	3,4-DICHLOROBENZENESULFONAMIDE 23815-28-3
9 *	3.85	1140		C6H5Cl5	PENTACHLOROCYCLOHEXENE-3,4,6/5 54083-25-9
1290 *	3.60	1140		C6H5Cl5	PENTACHLOROCYCLOHEXENE-3,4/5,6 54083-24-8
1 *	3.80	1140		C6H5Cl5	PENTACHLOROCYCLOHEXENE-3,5,6/4 51795-30-3
2 *	3.61	1140		C6H5Cl5	PENTACHLOROCYCLOHEXENE-3,5/4,6 643-15-2
3 *	3.95	1140		C6H5Cl5	PENTACHLOROCYCLOHEXENE-3,6/4,5 319-94-8
4 *	2.27	501		C6H5F1	FLUOROBENZENE 462-06-6
95	-0.68	7.4	2270	1 C6H5F1N2O3	5-FLUOROURACIL-3-ACETYL 75410-15-0
6 *	-0.34	4.0	2270	302	5-FLUOROURACIL-3-ACETYL
7	-1.38	7.4	2286	1 C6H5F1N2O4	URACIL,1-METHOXYCARBONYL-5-FLUORO 71759-43-8
8 *	-0.68	4.0	2010	"	URACIL,1-METHOXYCARBONYL-5-FLUORO
9 *	1.93	501		C6H5F1O1	M-FLUOROPHENOL 372-20-3
1300 *	1.71	501		C6H5F1O1	O-FLUOROPHENOL 367-12-4
1 *	1.77	501		C6H5F1O1	P-FLUOROPHENOL 371-41-5
2 *	1.54	1772		C6H5F2N1	2,4-DIFLUOROANILINE 367-25-9
3 *	3.36	536		C6H5F5S1	PHENYLSULFURPENTAFUORIDE 2557-81-5
4 *	3.25	508		C6H5I1	IODOBENZENE 591-50-4
5 *	-1.61	508		C6H5I1O1	IODOBENZENE 536-80-1
6 *	2.93	501		C6H5I1O1	M-IODOPHENOL 628-02-8
7 *	2.65	501		C6H5I1O1	O-IODOPHENOL 533-58-4
8 *	2.91	501		C6H5I1O1	P-IODOPHENOL 540-38-5
9 *	-1.33	541		C6H5I1O2	IODOXYBENZENE
1310 *	0.85	1478		C6H5N1O1	2-CYANOMETHYLFURAN 2745-25-7
1 *	2.01	508		C6H5N1O1	NITROSOBENZENE 586-98-9
2 *	0.44	594	400	C6H5N1O1	PYRIDINE,2-CARBOXYALDEHYDE 1121-60-4
3	0.14	594		C6H5N1O1	PYRIDINE,3-CARBOXYALDEHYDE 500-22-1
4	0.29	2247	459	"	PYRIDINE,3-CARBOXYALDEHYDE
15 *	0.43	547		C6H5N1O1	PYRIDINE-4-CARBOXYALDEHYDE 872-95-5
6	-1.15	3.8	547	C6H5N1O2	ISONICOTINIC ACID 55-22-1
7	-0.57	547	827	"	ISONICOTINIC ACID
6 *	1.08	536		C6H5N1O2	N-HYDROXYBENZOQUINONEMONIMINE 637-62-7
9	-0.82	4.5	2107	537 C6H5N1O2	NICOTINIC ACID 59-67-6 vitamin
1320	-0.66	3.0	2107	537	NICOTINIC ACID
1	-0.46	1135	537	"	NICOTINIC ACID
2	0.66	2.0	2312	337	NICOTINIC ACID
3 *	1.85	501		C6H5N1O2	NITROBENZENE 98-95-3
4 *	1.29	547		C6H5N1O2	P-NITROSOPHENOL 104-91-6
25	-1.98	2.0	447	C6H5N1O2	PICOLINIC ACID 98-98-6
6	-1.50	7.4	447	1	PICOLINIC ACID
7 *	1.98	1478		C6H5N1O2S1	2-(B-NITROVINYL)THIOPHENE 874-84-0
8 *	1.94	1478		C6H5N1O2S1	3-(B-NITROVINYL)THIOPHENE 28783-31-5
9 *	1.56	1478		C6H5N1O3	2-(B-NITROVINYL)FURAN 699-18-3
1330 *	1.41	1478		C6H5N1O3	3-(B-NITROVINYL)FURAN 53916-74-8
1	-2.53	7.4	447	1 C6H5N1O3	3-HYDROXPICOLINIC ACID 874-24-8
2	-1.27	2.0	447	"	3-HYDROXPICOLINIC ACID
3	1.74	7.4	2646	448 C6H5N1O3	M-NITROPHENOL 554-84-7
4 *	2.00	501		"	M-NITROPHENOL
35	1.68	7.4	2646	448 C6H5N1O3	O-NITROPHENOL 88-75-5
6 *	1.79	501		"	O-NITROPHENOL
7	1.36	7.4	772	1 C6H5N1O3	P-NITROPHENOL 100-02-7
8	1.77	7.4	2646	448	P-NITROPHENOL
9 *	1.91	501		"	P-NITROPHENOL
1340 ✓	-1.31	12.8	534	1 C6H5N1O3	SODIUM P-NITROPHENOXIDE 14609-74-6
1	-0.84	10.2	534	310	SODIUM P-NITROPHENOXIDE
2 *	1.66	1.0	594	C6H5N1O4	1,2-DIHYDROXIBENZENE,4-NITRO 3316-09-4
3 *	1.56	1.4	536	342 C6H5N1O4	2-NITRORESORCINOL 601-89-8
4	1.05	6.8	448	2 C6H5N1O4	4-NITRORESORCINOL 3163-07-3
45 *	-0.14	731	604	C6H5N1O4	N-MALEOYLGLYCINE 25021-08-3
6 *	1.26	1478		C6H5N1S1	2-CYANOMETHYLTHIOPHENE 20893-30-5
7 *	1.26	1478		C6H5N1S1	3-CYANOMETHYLTHIOPHENE 13781-53-8
8 *	0.30	594		C6H5N3	1H-IMIDAZO-[4,5-B]-PYRIDINE 273-21-2
9 *	0.18	2031		C6H5N3	5-PYRIDOIMIDAZOLE 272-97-9
1350 *	1.44	559		C6H5N3	BENZOTRIAZOLE 95-14-7
1 *	2.59	541		C6H5N3	PHENYLAZIDE 622-37-7
2 *	0.26	2499		C6H5N3	PYRAZINE,2-CYANO-5-METHYL
3 *	0.44	2499		C6H5N3	PYRAZINE,2-CYANO-6-METHYL
4	0.88	897	459	C6H5N3O1	2-PYRIDINENITRILE,4-METHOXY
55 *	0.89	2592		C6H5N3O1	BENZOTRIAZOLE,2-HYDROXY
6 *	0.95	2499		C6H5N3O1	PYRAZINE,2-CYANO-6-METHOXY
7 *	0.52	7.4	2206	306 C6H5N3O2	IMIDAZOLE,5-NITRO-1-PROPARGYL
8 *	1.79	547		C6H5N3O4	ANILINE,2,6-DINITRO 606-22-4
9 *	1.89	547		C6H5N3O4	ANILINE,3,5-DINITRO 618-87-1
1360 *	0.93	1002		C6H5N3O5	PICRAMIC ACID 96-91-3
1	0.96	332	1	C6H5N3S1	THIENO(2,3-D)-PYRIDINE,4-AMINO 14080-56-9 +
2	-1.10	1375		C6H5N5O2	1,2,4-TRIAZOLO(4,3-B)PYRIDAZIN-8-ONE-6-ME-7-OH-IMINYL +
3 *	2.24	579	400	C6H6	2,4-HEXADIENE 2809-69-0
4 *	2.13	501		C6H6	BENZENE 71-43-2

logP	pH	Ref. Note	MF	Name / CAS / activity
65	2.03	1734	C6H6	HEXADEUTEROBENZENE 1076-43-3
6 ★	3.28	421	456 C6H6Br1Cl4F1	2-F-3-BR-TETRACL-CYCLOHEXANE(2,3,5,6/1,4)
7 ★	3.81	421	456 C6H6Br1Cl5	1-BR-PENTACL-CYCLOHEXANE(2,3,5,6/1,4)
8 ★	3.74	421	456 C6H6Br1Cl5	2-BR-PENTACL-CYCLOHEXANE(2,3,5,6/1,4)
9 ★	2.10	272	C6H6Br1N1	M-BROMOANILINE 591-19-5
1370 ★	2.11	558	C6H6Br1N1	O-BROMOANILINE 615-36-1
1 ★	2.28	272	C6H6Br1N1	P-BROMOANILINE 106-40-1
2 ★	1.39	2.1	2265 C6H6Br1N1O2S1	BENZENESULFONAMIDE,3-BR
3 ★	1.36	2.0	264 C6H6Br1N1O2S1	P-BROMOBENZENESULFONAMIDE 701-34-8
4 ★	0.25	7.4	725 1 C6H6Br1N3O1	2-BROMOISONIAZID 29849-15-8
75 ★	3.88	421	456 C6H6Br2Cl4	1,2-DIBR-TETRACL-CYCLOHEXANE(2,3,5,6/1,4)
6 ★	3.99	421	456 C6H6Br2Cl4	2,3-DIBR-TETRACL-CYCLOHEXANE(2,3,5,6/1,4)
7 ★	1.68	501	C6H6Cl1N1	M-CHLOROANILINE 108-42-9
8 ★	1.90	530	C6H6Cl1N1	O-CHLOROANILINE 95-51-2
9	1.83	7.4	1737 1 C6H6Cl1N1	P-CHLOROANILINE 106-47-8
1380 ★	1.88	2293	400	P-CHLOROANILINE
1 ★	1.81	2163	459 C6H6Cl1N1O1	PHENOL,2-AMINO-4-CHLORO 95-85-2
2 ★	1.29	2.0	264 C6H6Cl1N1O2S1	M-CHLOROBENZENESULFONAMIDE 17260-71-8
3 ★	0.74	2.0	264 C6H6Cl1N1O2S1	O-CHLOROBENZENESULFONAMIDE 6961-82-6
4 ★	1.24	7.2	2036 1 C6H6Cl1N1O2S1	P-CHLOROBENZENESULFONAMIDE 98-64-6
85 ★	0.11	7.4	725 1 C6H6Cl1N3O1	2-CHLOROISONIAZID 58481-04-2
6 ★	0.56	2499	C6H6Cl1N3O1	PYRAZINE,2-ACETYLAMINO-5-CHLORO
7 ★	1.10	2499	C6H6Cl1N3O1	PYRAZINE,2-CHLORO-6-ACETYLAMINO
8 ★	2.00	594	C6H6Cl2N2	O-PHENYLENEDIAMINE,4,5-DICHLORO 5348-42-5
9 ★	3.65	1553	C6H6Cl4	TETRACHLOROCYCLOHEXENE(3/45)
1390 ★	3.52	1553	C6H6Cl4	TETRACHLOROCYCLOHEXENE(34/5)
1 ★	3.72	1553	C6H6Cl4	TETRACHLOROCYCLOHEXENE(35/4)
2 ★	3.74	1140	C6H6Cl4	TETRACHLOROCYCLOHEXENE
3 ★	3.08	1140	*	TETRACHLOROCYCLOHEXENE 1782-00-0
4 ★	3.08	1140	*	TETRACHLOROCYCLOHEXENE 319-81-3
95 ★	3.15	1140	*	TETRACHLOROCYCLOHEXENE 33875-95-5
6 ★	3.40	1140	*	TETRACHLOROCYCLOHEXENE 41992-55-6
7 ★	0.58	564	C6H6Cl4N2P11	DICHLORO-4,5-DICHLORO-O-PHENYLENEDIAMINOPLATINUM
8 ★	3.19	421	456 C6H6Cl5F1	2-FLUOROPENTACHLORO-CYCLOHEXANE(2,3,5,6/1,4)
9 ★	3.96	421	456 C6H6Cl5F1	1-iodo-penta-cl-cyclohexane(2,3,5,6/1,4)
1400 ★	4.05	421	456 C6H6Cl5I1	3-iodo-pentACL-CYCLOHEXANE(2,3,5,6/1,4)
1 ★	3.80	516	C6H6Cl6	HEXACHLOROCYCLOHEXANE, ALPHA ISOMER 319-84-8
2 ★	3.78	516	C6H6Cl6	HEXACHLOROCYCLOHEXANE, BETA ISOMER 319-85-7
3 ★	4.14	516	C6H6Cl6	HEXACHLOROCYCLOHEXANE, DELTA ISOMER 319-86-8
4 ★	3.72	421	C6H6Cl6	LINDANE 58-89-9 antiparasitic (topical)
5 ★	1.30	501	C6H6F1N1	M-FLUOROANILINE 372-19-0
6 ★	1.28	272	C6H6F1N1	O-FLUOROANILINE 348-54-9
7 ★	1.15	501	C6H6F1N1	P-FLUOROANILINE 371-40-4
8	-0.11	7.4	725 1 C6H6F1N3O1	2-FLUOROISONIAZID 369-24-4
9 ★	-0.20	4.0	2009 C6H6F1N3O3	URACIL,1-METHYLAMINOCARBONYL-5-FLUORO
1410 ★	2.32	558	C6H6I1N1	O-iodoaniline 615-43-0
1 ★	2.34	572	C6H6I1N1	P-iodoaniline 540-37-4
2	0.52	7.4	725 1 C6H6I1N3O1	2-iodoisoniazid 29247-87-8
3 ★	1.62	2.1	2265 C6H6I1O2S1	BENZENESULFONAMIDE,3-iodo
4 ★	1.59	2.1	2265 C6H6I1O2S1	BENZENESULFONAMIDE,4-iodo 825-86-5
15 ★	0.15	2412	C6H6N2O1	2-PYRIDINECARBOXAMIDE 1452-77-3
6 ★	-0.28	1519	400 C6H6N2O1	I-NICOTINAMIDE 1453-82-3
7	-0.44	7.2	2317 1 C6H6N2O1	NICOTINAMIDE 98-92-0 vitamin
8 ★	-0.37	547	C6H6N2O1	NICOTINAMIDE
9 ★	-0.34	1519	400	NICOTINAMIDE
1420 ★	0.20	2412	C6H6N2O1	PYRAZINE,2-ACETYL
1	0.68	7.2	2317 1 C6H6N2O1	PYRIDINE-3-ALDOXIME 1193-92-8
2 ★	0.77	579	C6H6N2O1	PYRIDINE-4-ALDOXIME 696-54-8
3	0.03	1456	C6H6N2O2	2-AMINO-4-NITROSOPHENOL
4 ★	0.99	163	459 C6H6N2O2	2-METHYL-5-NITROPYRIDINE 21203-68-0
25 ★	-0.17	1519	400 C6H6N2O2	2-PYRAZINECARBOXYLIC ACID,METHYL ESTER 6164-79-0
6 ★	0.65	7.4	447 1 C6H6N2O2	3-HYDROXYPICOLINAMIDE 933-90-4
7 ★	1.49	594	400 C6H6N2O2	BENZOQUINONE,1,4-DIOXIME 105-11-3
8 ★	1.37	501	C6H6N2O2	M-NITROANILINE 99-09-2
9 ★	1.85	547	C6H6N2O2	O-NITROANILINE 88-74-4
1430 ★	1.30	7.4	2646	P-NITROANILINE 100-01-6
1 ★	1.39	501	C6H6N2O2	P-NITROANILINE
2 ★	-0.43	2412	C6H6N2O2	PYRIDAZINE-3-CARBOXYLIC ACID,METHYL ESTER
3 ★	-0.27	2412	C6H6N2O2	PYRIDAZINE-4-CARBOXYLIC ACID,METHYL ESTER
4 ★	-0.71	2412	C6H6N2O2	PYRIMIDINE,2-METHOXYCARBONYL 34253-03-7
35 ★	-0.27	2412	C6H6N2O2	PYRIMIDINE-4-CARBOXYLIC ACID,METHYL ESTER
6 ★	0.03	2412	C6H6N2O2	PYRIMIDINE-5-CARBOXYLIC ACID,METHYL ESTER
7 ★	1.12	547	C6H6N2O2S1	1,3-DIHYDRO-BENZOTHIADIAZOLE-2,2-DIOXIDE 1615-06-1
8 ★	1.53	579	C6H6N2O3	2-AMINO-4-NITROPHENOL 99-57-0
9 ★	0.96	1909	C6H6N2O3	4-AMINO-2-NITROPHENOL 119-34-8
1440 ★	1.55	594	C6H6N2O3	PYRIDINE,2-METHOXY-5-NITRO 5446-92-4
1	0.63	2447	C6H6N2O4	4-PYRIMIDINECARBOXYLIC ACID,TETRAHYDRO-2,6-DIOXO,METHYL ESTER 6153-44-2
2 ★	0.55	2.0	264 C6H6N2O4S1	M-NITROBENZENESULFONAMIDE 121-52-8
3 ★	0.34	2.0	264 C6H6N2O4S1	O-NITROBENZENESULFONAMIDE 5455-59-4
4 ★	0.64	2.0	264 C6H6N2O4S1	P-NITROBENZENESULFONAMIDE 6326-93-5
45 ★	1.24	1519	C6H6N2S1	2-PYRIDINETHIOCARBOXAMIDE 5348-38-3
6 ★	0.67	1519	400 C6H6N2S1	3-PYRIDINETHIOCARBOXAMIDE 4821-86-3
7	-0.21	1375	C6H6N4O1	1,2,4-TRIAZOLO(4,3-B)PYRIDAZINE-6-ME-8-OH +
8 ★	-0.07	7.4	2206 306 C6H6N4O2	ACETONITRILE,2-METHYL-5-NITROIMIDAZOL-2YL
9 ★	-0.27	3.0	2191 C6H6N4O2	XANTHINE,1-METHYL 6136-37-4

	logP	pH	Ref. Note	MF	Name / CAS / activity	
1450	★	-0.72	2537	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>	XANTHINE,3-METHYL 1076-22-8	
1	★	-0.89	3.0	2191	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub>	XANTHINE,7-METHYL 552-62-5
2	★	1.70	811	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>2</sub> S <sub>2</sub>	1-(5-NO <sub>2</sub> -2-THIAZOLYL)-2-IMIDAZOLIDINETHIONE	
3	★	-0.76	7.4	725	1 C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	2-NITROISONIAZID 58481-05-3
4	★	-0.57	3.0	2191	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	URIC ACID,1-METHYL 708-79-2
55	★	-1.08	3.0	2191	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	URIC ACID,3-METHYL 605-99-2
6	★	-1.16	3.0	2191	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub>	URIC ACID,7-METHYL 812-37-3
7	★	0.93	7.4	2206	306 C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S <sub>1</sub>	1-(5-NO <sub>2</sub> -2-THIAZOLYL)-2-IMIDAZOLIDINONE 61-57-4 antischistosomal
8	★	0.95	555	"	"	1-(5-NO <sub>2</sub> -2-THIAZOLYL)-2-IMIDAZOLIDINONE
9	★	0.57	7.4	553	1 C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S <sub>1</sub>	2(1,3-OXAZOLIDINYLIDEN-2N)-5-NO <sub>2</sub> -THIAZOLE
1480	★	1.64	1731	C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>3</sub> S <sub>1</sub>	5-NITRO-2-FURALDEHYDETHIOSEMICARBAZONE	
1	★	1.46	7.4	595	1 C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	2,4-DINITROPHENYLHYDRAZINE 119-26-6
2	★	1.48	547	"	"	2,4-DINITROPHENYLHYDRAZINE
3	★	0.23	7.4	1497	1 C <sub>8</sub> H <sub>8</sub> N <sub>4</sub> O <sub>4</sub>	NITROFURAZONE 59-87-0 antinfecive (topical)
4	★	0.23	7.4	1022	1	NITROFURAZONE
65	★	0.62	7.4	772	1 C <sub>6</sub> H <sub>6</sub> O <sub>1</sub>	PHENOL 108-95-2
6	★	1.46	501	"	"	PHENOL
7	★	1.25	1478	C <sub>8</sub> H <sub>6</sub> O <sub>1</sub> S <sub>1</sub>	2-ACETYLTHTIOPHENE 88-15-3	
8	★	1.24	1478	C <sub>8</sub> H <sub>6</sub> O <sub>1</sub> S <sub>1</sub>	3-ACETYLTHTIOPHENE 1468-83-3	
9	★	0.52	1478	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	2-ACETYLFURAN 1192-62-7	
1470	★	0.67	1006	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	5-METHYLFURFURAL 620-02-0	
1	★	0.80	501	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	M-DIHYDROXYBENZENE 108-46-3 keratolytic	
2	★	0.86	508	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	O-DIHYDROXYBENZENE 120-80-9	
3	★	0.59	516	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	P-DIHYDROXYBENZENE 123-31-9 deipagmentor	
4	✓	-3.54	547	820 C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> S <sub>1</sub>	BENZENESULFINIC ACID,SODIUM SALT 873-55-2	
75	★	1.76	1478	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> S <sub>1</sub>	THIOPHEN-3-CARBOXYLIC ACID,METHYL ESTER 22913-26-4	
6	★	0.68	2163	459 C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	1,2,3-TRIHYDROXYBENZENE 87-68-1	
7	★	0.16	1.4	536	342 C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	1,3,5-TRIHYDROXYBENZENE 108-73-6 antispasmodic
8	★	1.28	2523	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	FURAN,3-METHOXYCARBONYL	
9	★	1.00	1055	C <sub>8</sub> H <sub>6</sub> O <sub>3</sub>	FUROIC ACID,METHYL ESTER 611-13-2	
1480	★	2.52	536	C <sub>8</sub> H <sub>6</sub> S <sub>1</sub>	THIOPHENOL 108-98-5	
1	★	0.06	541	606 C <sub>6</sub> H <sub>7</sub> As <sub>1</sub> O <sub>3</sub>	PHENYLARSONIC ACID 98-05-5	
2	★	1.58	502	C <sub>8</sub> H <sub>7</sub> B <sub>1</sub> O <sub>2</sub>	PHENYLBORONIC ACID 98-80-6	
3	★	-2.91	7.4	921	22 C <sub>8</sub> H <sub>7</sub> Br <sub>1</sub> N <sub>1</sub> I <sub>1</sub>	3-BROMO-N-METHYLPYRIDINIUM IODIDE 32222-42-7
4	★	0.46	579	C <sub>8</sub> H <sub>7</sub> Br <sub>1</sub> N <sub>2</sub>	P-BROMOPHENYLHYDRAZINEHCL 589-21-9	
85	★	1.39	13.0	579	224	"
6	★	-0.30	1584	C <sub>8</sub> H <sub>7</sub> Br <sub>1</sub> N <sub>2</sub> O <sub>3</sub>	P-BROMOPHENYLHYDRAZINEHCL	
7	★	1.02	2200	C <sub>8</sub> H <sub>7</sub> Br <sub>2</sub> N <sub>3</sub> O <sub>4</sub>	PYRIMIDINE-2,4-DIONE,3-METHOXY-5-BROMO-6-METHYL 77317-65-8	
8	★	0.85	1909	C <sub>8</sub> H <sub>7</sub> Cl <sub>1</sub> N <sub>2</sub>	MISONIDAZOLE,4,5-DIBROMO	
9	★	1.28	7.4	594	314 C <sub>6</sub> H <sub>7</sub> Cl <sub>1</sub> N <sub>2</sub>	4-CHLORO-M-PHENYLENEDIAMINE 5131-60-2
					O-PHENYLENEDIAMINE,4-CHLORO 95-83-0	
1490	★	1.50	2499	C <sub>8</sub> H <sub>7</sub> Cl <sub>1</sub> N <sub>2</sub>	PYRAZINE,3-CHLORO-2,5-DIMETHYL	
1	★	1.99	2499	C <sub>8</sub> H <sub>7</sub> Cl <sub>1</sub> N <sub>2</sub> O <sub>1</sub>	PYRAZINE,2-CHLORO-5-ETHOXY	
2	★	2.22	2499	C <sub>8</sub> H <sub>7</sub> Cl <sub>1</sub> N <sub>2</sub> O <sub>1</sub>	PYRAZINE,2-CHLORO-6-ETHOXY	
3	★	0.50	564	C <sub>8</sub> H <sub>7</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub> P <sub>1</sub>	DICHLORO-4-NITRO-O-PHENYLENEDIAMINOPLATINUM	
4	★	2.84	1553	C <sub>8</sub> H <sub>7</sub> Cl <sub>3</sub>	TRICHLOROCYCLOHEXENE(3/4/5) 56994-25-3	
95	★	0.45	564	C <sub>8</sub> H <sub>7</sub> Cl <sub>3</sub> N <sub>2</sub> P <sub>1</sub>	DICHLORO-4-CHLORO-O-PHENYLENEDIAMINOPLATINUM	
6	★	3.53	421	C <sub>8</sub> H <sub>7</sub> Cl <sub>5</sub>	1-H-PENTACHLOROCYCLOHEXANE 22138-39-2	
7	★	3.37	421	C <sub>8</sub> H <sub>7</sub> Cl <sub>5</sub>	3-H-PENTACHLOROCYCLOHEXANE	
8	★	2.54	421	C <sub>8</sub> H <sub>7</sub> Cl <sub>5</sub> O <sub>1</sub>	1-HYDROXPENTACHLOROCYCLOHEXANE 53861-64-6	
9	★	0.04	7.4	2361	1 C <sub>6</sub> H <sub>7</sub> F <sub>2</sub> N <sub>3</sub> O <sub>3</sub>	IMIDAZOLE,2-NITRO-1-(3-HYDROXY-2,2-DIFLUORO)PROPYL
1500	★	1.46	1501	100 C <sub>8</sub> H <sub>7</sub> F <sub>3</sub> N <sub>4</sub> O <sub>1</sub> S <sub>1</sub>	THIAZAFURON 25366-23-8	
1	★	1.85	1211	"	THIAZAFURON	
2	★	1.99	1695	C <sub>8</sub> H <sub>7</sub> F <sub>7</sub> N <sub>2</sub> S <sub>1</sub>	THIOUREA,N-2,3,4-HEPTAFLUOROBUTYL-N'-METHYL	
3	★	1.11	536	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub>	2-PICOLINE 109-06-8	
4	★	1.20	260	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub>	3-METHYLPYRIDINE 108-99-6	
5	★	1.22	260	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub>	4-METHYLPYRIDINE 108-99-4	
6	★	0.84	1734	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub>	PENTADEUTEROBENZAMINE 4165-61-1	
7	★	0.84	1734	"	PENTADEUTEROBENZAMINE 62-53-3	
8	★	0.90	501	"	PENTADEUTEROBENZAMINE	
9	★	0.95	7.4	1737	1	PENTADEUTEROBENZAMINE
1510	★	0.98	7.5	2201	"	PENTADEUTEROBENZAMINE
1	★	1.36	579	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	2-METHOXPYRIDINE 1628-89-3	
2	★	1.00	163	459 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	4-METHOXPYRIDINE 620-08-6	
3	★	0.06	1474	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	4-PYRIDINEMETHANOL 586-95-8	
4	★	0.21	5.6	726	41 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	M-AMINOPHENOL 591-27-5
15	★	-0.23	924	400 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	N-METHYL-A-PYRIDONE 694-85-9	
6	★	-1.22	924	400 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	N-METHYL-G-PYRIDONE 695-19-2	
7	★	-0.02	1474	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	NICOTINYL ALCOHOL 100-55-0 vasodilator (peripheral)	
8	★	0.62	508	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	O-AMINOPHENOL 95-55-6	
9	★	0.72	7.4	772	1	O-AMINOPHENOL
1520	★	0.04	7.4	772	1 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	P-AMINOPHENOL 123-30-8
1	★	0.04	531	"	"	P-AMINOPHENOL
2	★	0.79	541	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	PHENYLHYDROXYLAMINE 100-65-2	
3	★	0.06	1474	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	PICONOL 586-98-1	
4	★	0.99	2412	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	PYRIDINE,3-METHOXY 7295-76-3	
25	★	0.93	1625	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>1</sub>	PYRROLE,2-ACETYL 1072-63-9	
6	★	0.70	5.0	2153	2 C <sub>6</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub>	2-(1-PYRROLYL)ACETIC ACID
7	★	-0.49	7.4	2685	1 C <sub>6</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub>	4-PYRIDONE,3-HYDROXY-2-METHYL iron chelator
8	★	0.23	2523	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub>	FURAN-2-CARBOXAMIDE,N-METHYL	
9	★	0.34	2523	C <sub>6</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub>	FURAN-3-CARBOXAMIDE,N-METHYL	
1530	★	1.17	1625	457 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub>	PYRROLE-2-CARBOXYLIC ACID,METHYL ESTER 1193-62-0	
1	★	0.31	501	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub> S <sub>1</sub>	BENZENESULFONAMIDE 98-10-2	
2	★	-2.05	7.2	2323	466 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>2</sub> S <sub>1</sub>	THIENYLGLYCINE
3	★	-2.16	2457	300 C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>3</sub> S <sub>1</sub>	ANILINE-4-SULFONIC ACID 121-57-3 antibacterial	
4	★	0.48	590	C <sub>8</sub> H <sub>7</sub> N <sub>1</sub> O <sub>3</sub> S <sub>1</sub>	N-HYDROXYBENZENESULFONAMIDE 599-71-3	

logP	pH	Ref.	Note	MF	Name / CAS / activity
35 ★	0.06	5.6	726	41 C6H7N1O3S1	P-HYDROXYBENZENESULFONAMIDE 1576-43-8
6 ★	0.69	7.4	1022	1 C6H7N1O4	FURASPOR <i>antifungal</i>
7 ★	1.81	1478		C6H7N1S1	1-(THIOPHEN-2-YL)ACETALDEHYDEOXIME 59445-83-9
8 ★	1.10	1478		C6H7N1S1	2-ACETAMIDOTHIOPHENE 13053-81-1
9 ★	1.71	1519	459	C6H7N1S1	2-METHYLTHIOPYRIDINE 18436-38-5
1540 ★	0.31	1478		C6H7N1S1	3-ACETAMIDOTHIOPHENE 13781-66-3
1	1.43	7.4	547	1 C6H7N1S1	O-AMINOTHIOPHENOL 137-07-5
2 ★	0.33	1478		C6H7N1S1	THIOPHEN-2-YL-ACETAMIDE 4461-29-4
3 ★	1.31	594		C6H7N1S1	THIOPHENOL, 4-AMINO 1193-02-8
4 ★	-0.75	1519	400	C6H7N3O1	2-ACETAMIDOPYRIMIDINE 13053-88-8
45 ✓	0.88	7.0	538	701 C6H7N3O1	2-AMINONICOTINAMIDE 13438-65-8
6 ✓	0.70	7.0	538	701 C6H7N3O1	6-AMINONICOTINAMIDE 329-89-5
7	-1.14	7.4	725	1 C6H7N3O1	ISONIAZID 54-85-3 <i>antibacterial (tuberculostatic)</i>
8 ★	-0.70	1519	400		ISONIAZID
9 ★	-0.03	2412		C6H7N3O1	PYRAZINE, 2-ACETYLAMINO
1550 ★	-0.25	2499		C6H7N3O1	PYRAZINE, 2-CARBOXAMIDO-5-METHYL
1 ★	-0.13	2499		C6H7N3O1	PYRAZINE, 2-CARBOXAMIDO-6-METHYL
2 ★	-0.41	2412		C6H7N3O1	PYRIDAZINE, 4-ACETYLAMINO
3 ★	0.03	2412		C6H7N3O1	PYRIMIDINE, 4-ACETYLAMINO
4 ★	-0.22	2412		C6H7N3O1	PYRIMIDINE, 5-ACETYLAMINO
55 ★	0.64	7.4	1022	1 C6H7N3O2	1-METHYL-2-NITRO-5-VINYLMIDAZOLE
6 ★	0.53	1909		C6H7N3O2	2-NITRO-P-PHENYLENEDIAMINE 5307-14-2
7 ★	1.27	547		C6H7N3O2	3-NITRO-O-PHENYLENEDIAMINE 3894-52-8
8 ★	0.88	579		C6H7N3O2	4-NITRO-O-PHENYLENEDIAMINE 99-56-9
9 ★	0.62	7.4	2206	306 C6H7N3O2	IMIDAZOLE, 1-METHYL-5-NITRO-2-VINYL
1560 ★	1.41	13.0	594	C6H7N3O2	P-NITROPHENYLHYDRAZINE 100-16-3
1 ★	0.13	2499		C6H7N3O2	PYRAZINE, 2-CARBOXAMIDO-6-METHOXY
2 ★	-0.34	7.4	1022	1 C6H7N3O3	1-(ACETYLMETHYL)-2-NITROIMIDAZOLE
3 ★	-0.65	2352	2	C6H7N3O3S1	3-PYRIDINESULFONYLUREA
4 ★	-0.09	7.4	1022	1 C6H7N3O4	1-(CH2CO2CH3)-2-NITROIMIDAZOLE
65 ★	0.51	7.4	1022	1 C6H7N3O4	1-METHYL-2-NITRO-5-METHOXYCARBONYLMIDAZOLE
6	-1.70	7.4	2206	1 C6H7N3O4	ACETIC ACID, 2-METHYL-5-NITROIMIDAZOL-2YL 1010-93-1
7 ★	-0.03	7.4	2348	1 C6H7N5	ADENINE, 9-METHYL
8	-0.52	1375		C6H7N5O1	1,2,4-TRIAZOLO(4,3-B)PYRIDAZINE-6-ME-7-NH2-8-OH
9 ★	1.38	7.4	553	1 C6H7N5O2S1	2(1,3-IMIDAZOLINYLIDEN-2-AMINO)-5-NO2-THIAZOLE 24240-69-5
1570 ✓	-0.85	3.0	541	C6H7O3P1	PHENYLPHOSPHONIC ACID 1571-33-1
1 ★	0.54	3.0	541		PHENYLPHOSPHONIC ACID
2 ★	2.47	547	400	C6H8	1,3-CYCLOHEXADIENE 592-57-4
3 ★	2.30	547	400	C6H8	1,4-CYCLOHEXADIENE 628-41-1
4 ★	0.16	2200		C6H8Br1N3O4	MISONIDAZOLE, 5-BROMO
75 ★	2.12	7.4	1401	1 C6H8Cl1N1S1	CLOMETHIAZOLE 533-45-9 <i>sedative, tranquilizer</i>
6 ★	0.98	1519	400	C6H8Cl1N3	3-CHLORO-6-PYRIDAZINAMINE, N,N-DIMETHYL
7 ★	1.70	2499		C6H8Cl1N3	PYRAZINE, 2-CHLORO-6-DIMETHYLAMINO
8 ★	1.95	2499		C6H8Cl1N3	PYRAZINE, 2-CHLORO-6-DIMETHYLAMINO
9 ★	0.88	6.0	2417	1 C6H8Cl1N3O2	IMIDAZOLE, 1-CHLOROETHYL-2-METHYL-5-NITRO
1580	0.15	1008	354	C6H8Cl1N3O3	1(3-CL-2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
1	0.18	1467			1(3-CL-2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
2 ★	0.12	7.0	1783	1 C6H8Cl1N5O3	2-((6-AM-3-CL-5-NO2-PYRAZIN-2YL)AMINO)ETHANOL 86845-62-7
3 ★	-0.85	564		C6H8Cl2N2P11	DICHLORO-O-PHENYLENEDIAMINOPLATINUM
4 ★	2.82	421		C6H8Cl4	TETRACHLOROCYCLOHEXANE 60067-92-7
85 ★	-0.52	2354		C6H8F1N3O3	1-(3-FLUORO-2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
6	-0.44	7.4	2361	1	1-(3-FLUORO-2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
7	-0.39	7.4	1022	1	1-(3-FLUORO-2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
8 ★	-0.38	7.4	2361	1 C6H8F1N3O3	IMIDAZOLE, 2-NITRO-1-(3-HYDROXY-2-FLUORO)PROPYL
9 ✓	-3.30	7.4	921	22 C6H8N1,11	N-METHYLPYRIDINIUM IODIDE 930-73-4
1590 ★	0.63	163	459	C6H8N2	2,5-DIMETHYLPYRAZINE 123-32-0
1 ★	1.07	547		C6H8N2	2-(METHYLAMINO)PYRIDINE 4597-87-9
2 ★	0.56	7.0	566	1 C6H8N2	2-AMINO-4-PICOLINE 695-34-1
3 ★	1.02	260		C6H8N2	2-AMINO-5-METHYLPYRIDINE 1803-41-4
4 ★	0.69	2444		C6H8N2	2-ETHYLPYRAZINE
95 ★	-0.21	1474		C6H8N2	2-PYRIDINEMETHANEAMINE
6	-1.67	2.7	1473	340 C6H8N2	3-PYRIDINEMETHANEAMINE HYDROCHLORIDE
7 ★	0.62	260		C6H8N2	4,6-DIMETHYLPYRIMIDINE 1558-17-4
8	-1.51	2.7	1473	C6H8N2	4-PYRIDINEMETHANEAMINE HYDROCHLORIDE 3731-53-1
9 ★	-0.38	1474		C6H8N2	4-PYRIDINEMETHANEAMINE
1600 ★	-0.32	2069		C6H8N2	HEXANEDINITRILE 111-89-3
1 ★	-0.33	7.4	594	314 C6H8N2	M-PHENYLENEDIAMINE 108-45-2
2 ★	0.15	531		C6H8N2	O-PHENYLENEDIAMINE 95-54-5
3	-0.75	7.4	579	1 C6H8N2	P-PHENYLENEDIAMINE 624-18-0
4 ★	-0.30	1909			P-PHENYLENEDIAMINE
5 ★	1.25	8.9	534	2 C6H8N2	PHENYLHYDRAZINE 100-63-0
6 ★	-0.32	1474		C6H8N2	PICOLAMINE 3731-52-0
7 ★	0.54	2499		C6H8N2	PYRAZINE, 2,3-DIMETHYL
8 ★	0.54	2499		C6H8N2	PYRAZINE, 2,6-DIMETHYL 108-50-9
9 ★	0.35	594	400	C6H8N2	PYRAZOLE, 1-ALLYL
1610	-0.51	7.4	2362	1 C6H8N2	PYRIDINE, 3-METHYL-4-AMINO
1	-1.56	2.7	1473	340 C6H8N2	PYRIDINEMETHANEAMINEHYDROCHLORIDE 3731-51-9
2 ★	1.28	2412		C6H8N2O1	PYRAZINE, 2-ETHOXY
3 ★	1.24	2499		C6H8N2O1	PYRAZINE, 2-METHOXY-3-METHYL
4 ★	1.29	2499		C6H8N2O1	PYRAZINE, 2-METHYL-6-METHOXY
15 ★	0.63	2412		C6H8N2O1	PYRIDAZINE, 3-ETHOXY
6 ★	0.20	2412		C6H8N2O1	PYRIDAZINE, 4-ETHOXY
7	-0.06	7.4	2362	1 C6H8N2O1	PYRIDINE, 3-METHOXY-4-AMINO
8 ★	0.74	2412		C6H8N2O1	PYRIMIDINE, 2-ETHOXY
9 ★	0.97	2412		C6H8N2O1	PYRIMIDINE, 4-ETHOXY

	logP	pH	Ref. Note	MF	Name / CAS / activity
1620	★ 0.56		2412	C6H8N2O1	PYRIMIDINE,5-ETHOXY
1	★ 1.14		2499	C6H8N2O2	PYRAZINE,2,5-DIMETHOXY
2	★ 1.58		2499	C6H8N2O2	PYRAZINE,2,6-DIMETHOXY
3	★ -0.54		594	C6H8N2O2	PYRIMIDINE,1,3-DIMETHYL-2,4-DIOXO 874-14-6
4	★ 0.22	5.9	590	C6H8N2O2S1	BENZENESULFONAMIDE,2-AMINO 3306-62-5
25	★ -0.14	3.5	547	1 C6H8N2O2S1	BENZENESULFONYL HYDRAZIDE 80-17-1
6	★ -0.38		2467	448 C6H8N2O2S1	M-AMINOBENZENESULFONAMIDE 98-18-0
7	★ 0.40		541	C6H8N2O2S1	PHENYL SULFAMIDE 15959-53-2
8	★ -0.89	7.5	652	1 C6H8N2O2S1	SULFANILAMIDE 63-74-1 <i>antibacterial</i>
9	★ -0.76	7.4	1737	1	SULFANILAMIDE
1630	★ -0.62	5.5	2265		SULFANILAMIDE
1	★ 0.50	1.0	2202	342 C6H8N2O2S1	THIOBARBITURIC ACID,5,5-DIMETHYL
2	★ -0.35	0.7	962	C6H8N2O3	BARBITURIC ACID,5-ETHYL 2518-72-1
3	★ -0.55		2467	C6H8N2O4S2	1,3-BENZENEDISULFONAMIDE 3701-01-7
4	★ -0.96	2.1	2265	C6H8N2O4S2	1,4-BENZENEDISULFONAMIDE 16983-45-6
35	★ 1.31		1358	C6H8N2O8	ISOSORBIDENITRATE 87-33-2 <i>vasodilator (coronary)</i>
8	★ 1.81		2499	C6H8N2S1	PYRAZINE,2-METHIO-3-METHYL
7	★ 1.85		1519	459 C6H8N2S2	3,8-DIMETHYLTHIOPYRIDAZINE
8	★ -0.98	7.4	725	1 C6H8N4O1	2-AMINOISONIAZID 58481-01-9
9	★ 0.08		871	C6H8N4O1	N-NITROSO-BIS(2-CYANOETHYL)AMINE
1640	★ 0.04	7.4	1022	1 C6H8N4O3	1-METHYL-2-NITRO-5-(CH=N(O)CH3)IMIDAZOLE
1	0.29	7.4	2561	1 C6H8N4O3	2-NITROIMIDAZOLE-1-(ACETALDOXIME-METHYL ETHER)
2	★ -0.23	1.0	2186	C6H8N4O3	PYRAZOLE,3-METHYL-4-NITRO-5-(N-METHYLCARBOXAMIDE)
3	★ -0.74	7.4	2561	1 C6H8N4O4	2-NITROIMIDAZOLE-1-(N-HYDROXY-N-METHYLACETAMIDO)
4	★ -1.15	7.4	2561	1 C6H8N4O4	2-NITROIMIDAZOLE-1-(N-HYDROXYPROPIONAMIDO)
45	★ -1.08	7.4	2561	1 C6H8N4O4	2-NITROIMIDAZOLE-1-(N-METHOXYACETAMIDO)
6	★ -0.37	7.4	2206	308 C6H8N4O4	5-NITROIMIDAZOLE,1-ME-2-(ME-CARBAMATE) 7681-76-7 <i>antiprotozoal</i>
7	0.81		1731	C6H8N4O5	1-(B-O2NO-ET)2-METHYL-5-NITROIMIDAZOLE
8	★ 0.98		1987	C6H8N4S1	THIOPHENE-2-CARBOXALDEHYDE, GUANYLHYDRAZONE 97183-52-3
9	★ 0.76	6.0	2417	1 C6H8N6O2	IMIDAZOLE,1-AZIDOETHYL-2-METHYL-5-NITRO
1650	★ 0.65	7.4	2206	308 C6H8N6O2S1	CARBOXALDEHYDETHIOSEMICARBAZONE,1-METHYL-5-NITROIMIDAZOL-2YL 4994-21-2
1	★ 0.58		513	C6H8O1	1-HEXYN-5-ONE
2	★ 0.61		1625	C6H8O1	2-CYCLOHEXENE-1-ONE 930-68-7
3	★ 2.40		1476	C6H8O1	2-ETHYLFURAN 3208-18-0
4	★ 2.24		2819	C6H8O1	FURANE,2,5-DIMETHYL 625-86-5
55	★ 1.33		1135	537 C6H8O2	SORBITIC ACID 110-44-1 <i>antimicrobial agent</i>
6	★ 0.04		1059	C6H8O3S1	5,6-DIHYDRO-2-METHYL-1,4-OXATHIIN-3-CARBOXYLIC ACID +
7	★ 0.74		579	C6H8O4	FUMARIC ACID,METHYL ESTER 624-49-7
8	★ 0.22		579	C6H8O4	MALEIC ACID,METHYL ESTER 624-48-6
9	★ -1.64	3.0	594	C6H8O6	ASCORBIC ACID 50-81-7 <i>vitamin (antiscorbutic)</i>
1660	★ -1.72		510	C6H8O7	CITRIC ACID 77-92-9 <i>acidifier, flavoring agent</i>
1	★ 2.87		1478	C6H8S1	2-ETHYLTHIOPHENE 872-55-9
2	★ 2.82		1478	C6H8S1	3-ETHYLTHIOPHENE 52006-63-0
3	★ -0.04	7.4	2361	1 C6H9F1N4O3	TRIAZINE,3-NITRO-1-(3-METHOXY-2-FLUORO)PROPYL
4	★ 2.31		2488	C6H9F2N5S1	1,3,5-TRIAZINE,2-DIFLUOROMETHIO-4,6-BIS-METHYLAMINO
65	★ 1.47		2819	C6H9N1	PYRROLE,2,5-DIMETHYL 625-84-3
8	★ 1.59		2619	C6H9N1	PYRROLE,2-ETHYL
7	★ 0.37		572	C6H9N1O1	N-VINYL-2-PYRROLIDINONE 86-12-0
8	★ -0.05	5.0	2425	1 C6H9N1O2	2-PYRROLIDONE,1-ACETYL 932-17-2
9	★ -0.70		213	C6H9N1O2	N-FORMYLCYCLOBUTANECARBOXAMIDE 23046-86-8
1670	★ -0.22		1059	C6H9N1O2S1	5,6-DIHYDRO-2-METHYL-1,4-OXATHIIN-3-CARBOXAMIDE +
1	★ -0.35		579	C6H9N1O2S1	CITIOLONE 1195-16-0 <i>treatment of hepatic disorder</i>
2	★ 0.36	7.4	2490	1 C6H9N1O3S3	THIOPHENE-2-SULFONAMIDE,5-HYDROXYETHYL 104437-96-9
3	★ -0.54	7.4	2490	1 C6H9N1O5S3	THIOPHENE-2-SULFONAMIDE,5-(HYDROXYETHYL)SULFONYL 104438-00-8
4	★ -0.40		2073	C6H9N1O6	ISOSORBIDE-2-NITRATE 16106-20-0 <i>vasodilator (coronary)</i>
75	★ -0.15		2073	C6H9N1O6	ISOSORBIDE-5-NITRATE 16051-77-7
6	★ 0.39		1519	C6H9N3	2,6-DIMETHYL-4-PYRIMIDINAMINE 461-88-3
7	★ 0.29		1519	400 C6H9N3	3-PYRIDAZINAMINE,N,N-DIMETHYL 17258-31-0
8	★ -0.32		1375	C6H9N3	3-PYRIDAZINEAMINE,4,6-DIMETHYL
9	★ -0.09		1519	459 C6H9N3	4-PYRIDAZINAMINE,N,N-DIMETHYL 17258-38-7
1680	★ 0.93		2412	C6H9N3	PYRAZINEAMINE,N,N-DIMETHYL 5214-29-9 <i>stimulant (central)</i>
1	0.98	7.4	579	1	PYRAZINEAMINE,N,N-DIMETHYL
2	★ -0.85	7.4	2362	1 C6H9N3	PYRIDINE,3-METHYLAMINO-4-AMINO
3	★ 1.07		2412	C6H9N3	PYRIMIDINE,2-DIMETHYLAMINO 5621-02-3
4	★ 0.58		2412	C6H9N3	PYRIMIDINE,4-DIMETHYLAMINO 31401-45-3
85	★ 0.48		2412	C6H9N3	PYRIMIDINE,5-DIMETHYLAMINO 31401-46-4
6	★ -0.85		1375	C6H9N3O1	3-AMINO-4-METHOXY-6-METHYLPYRIDAZINE
7	★ -3.58		1590	459 C6H9N3O2	HISTIDINE 71-00-1 <i>amino acid</i>
8	★ -1.95	7.0	1207	1	HISTIDINE
9	★ 0.62	7.4	2206	306 C6H9N3O2	IMIDAZOLE,2-ETHYL-1-METHYL-5-NITRO
1690	★ 0.76	7.4	2206	306 C6H9N3O2	IMIDAZOLE,2-ETHYL-4-METHYL-5-NITRO
1	★ -0.60	7.4	2206	306 C6H9N3O3	1-(2-OH-ETHYL)-2-METHYL-4-NITROIMIDAZOLE
2	★ -0.59		1008	354	1-(2-OH-ETHYL)-2-METHYL-4-NITROIMIDAZOLE
3	★ -0.16		1003	C6H9N3O3	1-(2-HYDROXYPROPYL)-2-NITROIMIDAZOLE
4	★ 0.12	7.4	1022	1 C6H9N3O3	1-(2-METHOXYMETHYL)-2-NITROIMIDAZOLE
95	★ -0.09		2387	C6H9N3O3	IMIDAZOLE,1,2-DIMETHYL-4-NITRO-5-METHOXY 35687-44-6
6	★ 0.18		2474	C6H9N3O3	IMIDAZOLE-1-ETHANOL,5-METHYL-2-NITRO 23571-38-2
7	★ -0.16	7.4	2380	1 C6H9N3O3	METRONIDAZOLE 443-48-1 <i>antiprotozoal (trichomonas)</i>
8	★ -0.11	7.4	694	1	METRONIDAZOLE
9	★ -0.09	7.4	2206	306	METRONIDAZOLE
1700	★ -0.02		1080		METRONIDAZOLE
1	★ -0.08	7.4	830	1 C6H9N3O3	N-DIAZOACETYLGLYCINE,ETHYL ESTER 999-29-1
2	★ -1.22		1467	C6H9N3O3S1	1-(2-METHYLSULFINYLETHYL)-2-NITROIMIDAZOLE
3	★ -0.96		1080	C6H9N3O4	1-(2,3-DIHYDROXYPROPYL)-2-NITROIMIDAZOLE 13551-92-3 <i>antineoplastic</i>
4	★ -0.89	7.4	1022	1 C6H9N3O4	1-METHYL-2-NITRO-5-(1,2-DIHYDROXYETHYL)IMIDAZOLE

logP	pH	Ref.	Note	MF	Name / CAS / activity
5	-0.37	2278		C6H9N3O4S1	IMIDAZOLE,1-METHYL-4-NITRO-5-ETHYLSULFONATO 13755-80-1
6 *	-1.30	1022	1	C6H9N3O4S1	METHYL(2-(2-NITRO-1-IMIDAZOLYL)ETHYL)SULFONE
7 *	0.02	536	342	C6H9N3O4S2	ANILINE,N-(SO2NH3O2NH2)
8	-2.05	2417	1	C6H9N3O5S1	IMIDAZOLE,1-ETHANESULFONIC ACID-2-METHYL-5-NITRO
9	-1.57	694	1	C6H9N3O5S2	IMIDAZOLE,2-METHYL-5-NITRO-1-(2-ETHYLTHIO)SULFONIC ACID, SODIUM SALT
1710 ✓	-1.01	1412		C6H9N5O2	1,2,4-TRIAZOLE,3,5-DIACETAMIDO
1 *	-1.59	2273	1	C6H9N5O4	(3-NITRO-1,2,4-TRIAZOL-1-YL)ACETAMIDE,N-(2-HYDROXY)ETHYL 104958-85-2
2 *	2.87	594	400	C6H10	1,5-HEXADIENE 592-42-7
3	2.73	1560	100	C6H10	1-HEXYNE 693-02-7
4 *	2.80	594	400	C6H10	CIS-2-TRANS-4-HEXADIENE 5194-50-3
15 *	2.86	547	400	C6H10	CYCLOHEXENE 110-83-8
6 *	3.16	594	400	C6H10	TRANS-1,3-HEXADIENE 592-48-3
7 *	3.01	594	400	C6H10	TRANS-2-TRANS-4-HEXADIENE 5194-51-4
8	-1.82	401	1	C6H10Cl1N3O4	UREA,1-(2CLET)-1-NO-3-(2-PROPIONIC ACID)
9	1.84	401	2		UREA,1-(2CLET)-1-NO-3-(2-PROPIONIC ACID)
1720	1.51	2550	459	C6H10Cl1N5	DESETHYLATRAZINE
1 *	3.18	1553		C6H10Cl2	1,2-DICHLOROCYCLOHEXANE-C
2 *	3.21	1553		C6H10Cl2	1,2-DICHLOROCYCLOHEXANE-TRANS
3 *	1.13	547		C6H10N2O1	4-I-PROPOXYPIRAZOLE
4 *	1.42	547		C6H10N2O1	4-PROPOXYPIRAZOLE
25 *	1.71	2186		C6H10N2O1	FURAZAN,METHYLPROPYL 77590-78-0
6 *	-0.68	1728		C6H10N2O2	N-NITROSOPIPERIDONE,3-METHYL
7 *	0.49	2188		C6H10N2O2S2	METHYLCARBAMIC ACID,2-OXIMINO-1,4-DITHIANE ESTER
8 *	0.91	2188		C6H10N2O2S2	METHYLCARBAMIC ACID,4-OXIMINO-5-METHYL-1,3-DITHIANE ESTER
9 *	0.00	2188		C6H10N2O3S1	METHYLCARBAMIC ACID,3-OXIMINO-1,4-OXATHIANE ESTER
1730 *	0.46	2188		C6H10N2O3S1	METHYLCARBAMIC ACID,4-OXIMINO-5-METHYL-1,3-OXATHIANE ESTER
1 *	-2.80	1591		C6H10N2O4	ASPARTIC ACID-MONOAMIDE,N-ACETYL
2	3.25	509		C6H10N2O6S3	IMIDAZOLE,2,4,5-TRIMETHYLSULFONYL 59800-83-0
3	-3.00	2003	314	C6H10N3O2.Cl1	IMIDAZOLIUM CHLORIDE,1-METHOXYMETHYL-2-HYDROXYIMINOMETHYL-3-METHYL 91900-09-3
4 *	0.14	953		C6H10N4	METRAZOLE 54-95-5 <i>cns stimulant, narcotic antagonist</i>
35 *	1.22	57		C6H10N4O1S1	3-MERCAPTO-4-AMINO-6-I-PROPYL-1,2,4-TRIAZIN-5-ONE 22278-77-9
6 *	0.46	57		C6H10N4O1S1	3-METHIO-4-AMINO-6-ETHYL-1,2,4-TRIAZINE-5-ONE 21087-59-2
7 *	-0.62	830	1	C6H10N4O2	N-DIAZOACETYLGLYCINE-N'-ETHYLAMIDE
8 *	-1.35	830	1	C6H10N4O3	N-DIAZOACETYLGLYCINE-N'-HYDROXYETHYLAMIDE
9 *	-0.49	2273	1	C6H10N4O4	1,2,4-TRIAZOLE,3-NITRO-1-(2-HYDROXY-3-METHOXY)PROPYL 104958-86-3
1740 *	-0.38	2587		C6H10N4O4	4-NITRO-1,2,3-TRIAZOLE,1-(N-(3-METHOXY-2-HYDROXY)PROPYL
1 *	-0.07	2587		C6H10N4O4	4-NITRO-1,2,3-TRIAZOLE,2-N-(3-METHOXY-2-HYDROXY)PROPYL
2 *	-0.12	563		C6H10N6O1	3-(3,3-DIMETHYL-1-TRIAZENO)PYRAZOLE-4-CARBOXAMIDE 21466-00-2
3 *	-0.24	525		C6H10N6O1	IMIDAZOLE,4-CARBOXAMIDE-5-(3,3-DIMETHYLTRIAZENYL) 4342-03-4 <i>antineoplastic</i>
4	1.26	1821	1	C6H10O1	1,2-EPOXYCYCLOHEXANE 286-16-8
45 *	1.02	502		C6H10O1	1-HEXEN-5-ONE 109-49-8
6 *	0.81	527		C6H10O1	CYCLOHEXANONE 108-94-1
7 *	-0.27	579		C6H10O2	2,5-HEXANEDIONE 110-13-4
8	0.46	2596		C6H10O2	ALLYL GLYCIDYL ETHER 106-92-3
9 *	1.94	1402		C6H10O2	METHACRYLIC ACID,ETHYL ESTER 97-63-2
1750 *	-0.13	502		C6H10O3	4-KETOVALERIC ACID,METHYL ESTER 624-45-3
1 *	0.35	1402		C6H10O3	ACRYLIC ACID,2-HYDROXYPROPYL ESTER 999-61-1
2 *	0.24	579		C6H10O3	ETHYLACETOACETATE 141-97-9
3 *	0.47	1402		C6H10O3	METHACRYLIC ACID,2-HYDROXYETHYL ESTER 888-77-9
4 *	-1.29	401		C6H10O4	1,2,5,6-DIANHYDROGALACTITOL 23281-20-3
55 *	0.08	510		C6H10O4	ADIPIC ACID 124-04-9
6 *	0.35	594		C6H10O4	BUTANEDIOIC ACID,METHYL ESTER 106-65-0
7 *	0.56	592		C6H10O4	OXALIC ACID,DIETHYL ESTER 95-92-1
8 *	-2.57	1144		C6H10O7	GLUCURONIC ACID 6556-12-3
9 ✓	-2.50	1986		C6H11Au1O5S1	GOLD THIOLUCOSE 12192-57-3 <i>antirheumatic</i>
1760 *	3.20	1683		C6H11Br1	BROMOCYCLOHEXANE 108-85-0
1 *	1.14	843		C6H11Br1N2O2	BROMISOVALUM 496-67-3 <i>sedative, hypnotic</i>
2 *	1.00	843		C6H11Cl1N2O2	A-CHLORO-I-VALERYLUREA
3 *	1.70	1942		C6H11F3O1	1,1,1-TRIFLUOROHXANOL-3
4 *	1.64	1942		C6H11F3O1	6,6,6-TRIFLUOROHXANOL
65 ✓	1.87	567	820	C6H11N1	DIALYLAMINE PICRATE
6 *	1.11	586	224	C6H11N1	DIALYLAMINE 124-02-7
7 *	1.66	1696		C6H11N1	HEXANENITRILE 628-73-9
8 *	1.54	1896		C6H11N1	I-HEXANENITRILE
9 *	-2.58	401		C6H11N1O2	1-AMINOCYCLOPENTANECARBOXYLIC ACID 52-52-8 <i>antineoplastic</i>
1770 *	-2.89	2654	448	C6H11N1O2	3-CARBOXYPIPERIDINE 498-95-3
1	-2.66	1207	1		3-CARBOXYPIPERIDINE
2 *	-3.05	2654	448	C6H11N1O2	4-CARBOXYPIPERIDINE
3 *	-2.31	2654	448	C6H11N1O2	HOMOPROLINE
4 *	1.09	504		C6H11N1O2	O-(1-ETHYL-ALLYL)CARBAMATE
75 *	-0.57	2228	314	C6H11N1O3	ALANINE-N-ACETYL,METHYL ESTER 3619-02-1
6 *	0.75	561		C6H11N1S1	2-AZACYCLOHEPTANTHIONE 7203-96-5
7 *	2.42	1693		C6H11N2O4P1S3	METHIDATHION 950-37-8 <i>insecticide</i>
8 *	0.65	1137		C6H11N3O1	2-AMINO-5-BUTYL-1,3,4-OXADIAZOLE 52836-38-7
9 *	0.40	1137		C6H11N3O1	2-AMINO-5-I-BUTYL-1,3,4-OXADIAZOLE
1780 *	0.62	1137		C6H11N3O1	2-AMINO-5-S-BUTYL-1,3,4-OXADIAZOLE
1 *	0.48	1137		C6H11N3O1	2-AMINO-5-T-BUTYL-1,3,4-OXADIAZOLE
2 *	-2.41	1591		C6H11N3O3	ASPARAGIN-AMIDE,N-ACETYL
3 *	0.36	536		C6H11N3O4	2-ME-2-NITROPROPIONALDEHYDE-N-ME-CARBAMOYLXIME 8129-11-9
4 *	-2.68	547	463	C6H11N3O4	GLY-GLY-GLY 556-33-2
85	0.16	723		C6H11N5O1	2,4-DIAMINO-6-DIMETHYLAMINO-PYRIMIDINE-3-OXIDE
6	-0.04	723		C6H11N5O1	2,4-DIAMINO-6-ETHYLAMINO-PYRIMIDINE-3-OXIDE
7 *	3.39	1560	100	C6H12	1-HEXENE 592-41-6
8 *	3.44	547	60	C6H12	CYCLOHEXANE 110-82-7
9 *	3.37	579		C6H12	METHYLCYCLOPENTANE 96-37-7

logP	pH	Ref. Note	MF	Name / CAS / activity
1790 ★	-0.29	401	C6H12Br2O4	1,6-DIBROMO-1,6-DIDEOXYGALACTITOL 10318-26-0 <i>antineoplastic</i>
1 ★	-0.24	401	C6H12Br2O4	NSC94100 488-41-5
2 ✓	1.53	1701	820 C6H12F3N1	N,N-DIETHYL-2,2,2-TRIFLUOROETHYLAMINE PICRATE
3 ★	1.88	1701	C6H12F3N1	N-ETHYL-2,2,2-TRIFLUOROETHYLAMINE 37174-09-7
4 ✓	1.78	1701	820 C6H12F3N1	N-PROPYL-N-METHYL-2,2,2-TRIFLUOROETHYLAMINE PICRATE
95 ★	2.18	1701	C6H12F3N1	N-PROPYL-N-METHYL-2,2,2-TRIFLUOROETHYLAMINE
6 ★	1.48	2506	C6H12N1O4P1S2	FORMOTHION 2540-82-1 <i>insecticide</i>
7	-1.93	532	820 C6H12N2O1	1-(2-HYDROXYETHYL)-2-METHYLIMIDAZOLINEHCL
8 ★	0.04	532	C6H12N2O1	1-(2-HYDROXYETHYL)-2-METHYLIMIDAZOLINE 696-94-3
9 ★	0.86	871	C6H12N2O1	2,5-DIMETHYL-N-NITROSOPYRROLIDINE 55556-86-0
1800 ★	0.71	871	C6H12N2O1	2-METHYL-N-NITROSOPIPERIDINE 7247-89-4
1 ★	0.99	871	C6H12N2O1	3-METHYL-N-NITROSOPIPERIDINE 13603-07-1
2 ★	1.05	871	C6H12N2O1	4-METHYL-N-NITROSOPIPERIDINE 15104-03-7
3 ★	0.92	871	C6H12N2O1	N-NITROSO-HEXAMETHYLENEIMINE 932-83-2
4 ★	0.32	871	C6H12N2O2	2,6-DIMETHYL-N-NITROSOMORPHOLINE 1456-28-6
5 ★	-1.21	1558	C6H12N2O2	ALANINE,N-ACETYL,N'-METHYLAMINO-AMIDE
6 ★	-0.87	7.0 2309	1 C6H12N2O2	GLYCINAMIDE,2,2-DIMETHYL-N-ACETYL
7 ★	0.45	673	C6H12N2O2	I-VALERYLUREA 2274-08-0
8 ★	-1.57	7.1 1591	C6H12N2O3	THREONIN-AMIDE,N-ACETYL
9 ★	0.73	594	400 C6H12N2S1	1-PIPERIDINETHIOCARBOXAMIDE 14294-09-8
1810 ★	-0.62	2083	C6H12N3O1P1	PHOSPHINEOXIDE,TRIS-(1-AZIRIDINYL) 545-55-1 <i>antineoplastic</i>
1 ★	0.53	401	C6H12N3P1S1	THIOTEPA 52-24-4 <i>antineoplastic</i>
2 ★	0.42	1705	C6H12N4	GUANIDINE,N1-PROPYL-N2-CYANO-N3-METHYL
3	1.29	3.5 2391	1 C6H12N4	TETRAZOLE,5-I-AMYL
4 ★	0.15	871	C6H12N4O2	2,5-DIMETHYL-N,N'-DINITROSOPIPERAZINE 55556-88-2
15 ★	0.08	871	C6H12N4O2	2,6-DIMETHYL-N,N'-DINITROSOPIPERAZINE 55380-34-2
6 ★	1.93	2219	C6H12O1	1,2-EPOXYHEXANE
7 ★	1.38	502	C6H12O1	2-HEXANONE 581-78-6
8 ★	1.31	2047	C6H12O1	4-METHYL-2-PENTANONE 108-10-1 <i>alcohol denaturant</i>
9 ★	1.23	503	C6H12O1	CYCLOHEXANOL 108-93-0
1820 ★	1.78	7.0 568	1 C6H12O1	HEXALDEHYDE 66-25-1
1 ★	1.20	579	400 C6H12O1	PINACOLONE 76-97-8
2 ★	1.22	1952	C6H12O1	TETRAHYDROFURAN,2,5-DIMETHYL (CIS) 2144-41-4
3 ★	1.34	1952	C6H12O1	TETRAHYDROFURAN,2,5-DIMETHYL (TRANS) 2390-94-5
4	1.90	3.5 2391	1 C6H12O2	2,2-DIMETHYLBUTYRIC ACID 595-37-9
25 ★	1.68	1815	C6H12O2	2-ETHYL-BUTANOIC ACID 88-09-5
6 ★	1.80	1815	C6H12O2	2-METHYL-PENTANOIC ACID 97-61-0
7 ★	1.78	594	400 C6H12O2	ACETIC ACID, BUTYL ESTER 123-86-4
8 ★	1.72	594	400 C6H12O2	ACETIC ACID, S-BUTYL ESTER 105-46-4
9 ★	1.76	594	400 C6H12O2	ACETIC ACID, T-BUTYL ESTER 540-88-6
1830 ★	0.23	508	C6H12O2	CYCLOHEXANEDIOL-CIS 1792-81-0
1 ★	0.08	508	C6H12O2	CYCLOHEXANEDIOL-TRANS 1460-67-7
2	1.98	1533	820 C6H12O2	HEXANOIC ACID, HEXYLAMINE SALT
3 ★	1.92	505	C6H12O2	HEXANOIC ACID 142-82-1
4 ★	1.78	594	400 C6H12O2	I-BUTYLACETATE 106-63-8
35	0.80	2596	C6H12O2	I-PROPYL GLYCIDYL ETHER 4016-14-2
6 ★	1.82	594	400 C6H12O2	ISOVALERIC ACID,METHYL ESTER
7	0.59	2596	C6H12O2	PROPYL GLYCIDYL ETHER 3126-95-2
8 ✓	-2.17	508	C6H12O2	SODIUM HEXANOATE
9 ★	1.83	594	400 C6H12O2	TRIMETHYLACETIC ACID,METHYL ESTER 598-98-1
1840 ★	1.96	594	400 C6H12O2	VALERIC ACID,METHYL ESTER 624-24-8
1	0.43	1266	C6H12O3	ETHYL-4-HYDROXYBUTYRATE 999-10-0
2 ★	0.67	7.5 1510	1 C6H12O3	PARALDEHYDE 123-63-7 <i>hypnotic, sedative</i>
3 ★	3.80	1560	100 C6H13Br1	1-BROMOHEXANE 111-25-1
4 ★	1.33	13.0 588	224 C6H13N1	ALLYLPROPYLAMINE 5666-21-7
45 ✓	2.47	587	820 C6H13N1	CYCLOHEXYLAMINE PICRATE
6 ★	1.49	13.0 588	224 C6H13N1	CYCLOHEXYLAMINE 108-91-8
7 ★	1.30	11.0 1443	322 C6H13N1	N-METHYLPYPERIDINE 626-87-5
8 ★	0.34	579	C6H13N1O1	DIETHYLACETAMIDE 685-91-6
9 ★	2.70	2571	C6H13N1O2	1-NITROHEXANE 646-14-0
1850 ★	-2.95	2018	C6H13N1O2	6-AMINOHEXANOIC ACID 60-32-2 <i>hemostatic</i>
1	-1.60	2323	468 C6H13N1O2	A-AMINOCAPROIC ACID 327-57-1
2 ★	-1.54	2654	448	A-AMINOCAPROIC ACID
3 ★	1.38	1969	C6H13N1O2	DIMETHYL CARBAMATE,I-PROPYL ESTER 38580-89-1
4 ★	-1.72	7.0 2197	C6H13N1O2	I-LEUCINE 73-32-5 <i>amino acid</i>
55	-1.61	7.0 2197	C6H13N1O2	LEUCINE 61-90-5 <i>amino acid</i>
6 ★	-1.52	405		LEUCINE
7 ★	1.35	7.4 172	1 C6H13N1O2	O-PENTYL CARBAMATE 638-42-6
8 ★	0.94	7.4 172	1 C6H13N1O2	O-T-PENTYL CARBAMATE
9 ★	-1.77	1233	C6H13N1O2	T-BUTYLGLYCINE 33105-81-8
1860 ★	0.73	871	C6H13N3O1	N-NITROSO-3,5-DIMETHYLPYPERAZINE
1 ★	1.11	871	C6H13N3O2	1-NITROSO-3,3-DIETHYL-1-METHYLUREA 50265-72-8
2	-3.19	1590	459 C6H13N3O3	CITRULLINE 372-75-8 <i>anti-asthenia</i>
3 ★	3.42	579	400 C6H14	2,3-DIMETHYLBUTANE 78-29-6
4 ★	3.90	1389	C6H14	HEXANE 110-54-3
65	3.82	547	400 C6H14	NEOHEXANE 75-83-2
6	-3.83	1257	820 C6H14N1O2.11	FORMYLCHOLINE IODIDE
7 ✓	-3.61	1704	820 C6H14N1O2.C2H3.Br1	(DEUTEROACETYL OXYME)TETRAMETHYLAMMONIUMBROMIDE
8 ✓	0.83	567	820 C6H14N1.C6H2N3O7	N,N-DIMETHYLPYRROLIDINIUM PICRATE
9 ★	0.08	594	C6H14N2	1-PYRROLIDINETHANAMINE 7154-73-6
1870 ★	-0.40	13.0 594	C6H14N2	N-METHYLHOMOPYPERAZINE 4318-37-0
1 ★	-0.40	13.0 594	400 C6H14N2	PIPERAZINE,1,4-DIMETHYL 106-58-1
2 ★	1.36	2570	C6H14N2O1	DI-I-PROPYLNITROSAMINE 601-77-4
3 ★	1.36	871	C6H14N2O1	DIPROPYLNITROSAMINE 621-84-7
4	1.57	2570	C6H14N2O1	ETHYLBUTYLNITROSAMINE 4549-44-4