Cyclobarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-cyclohexen-1-yl)-5-ethyl-
	5-(1-Cyclohexen-1-yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-(1-Cyclohexen-1-yl)-5-ethylbarbituric acid
	5-(1-Cyclohexenyl)-5-ethylbarbituric acid
	5-Ethyl-5-cyclohexenylbarbituric acid
	Adorm
	Amnosed
	Barbituric acid, 5-(1-cyclohexen-1-yl)-5-ethyl-
	Cavonyl
	Cyclobarbitol
	Cyclobarbiton
	Cyclobarbitone
	Cyclodorm
	Cyclohexal
	Cyclohexenyl-ethyl barbituric acid
	Cyklodorm
	Ethylhexabital
	Fanodorm
	Fanodormo
	Hexemal
	Hypnoval
	Irifan
	Namuron
	Palinum
	Phanodorm
	Phanodorn
	Philodorm
	Praelumin
	Pralumin
	Pro-Sonil
	Sonaform
	Sonoform
	Tetrahydrophenobarbital
Inchi:	InChI=1S/C12H16N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h6H,2-5,7H2,
InchiKey:	WTYGAUXICFETTC-UHFFFAOYSA-N
Formula:	C12H16N2O3
SMILES:	CCC1(C2=CCCCC2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	236.27
CAS:	52-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.74	kJ/mol	Joback Method
hf	-437.96	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-2.17		Aqueous Solubility Prediction Method
log10ws	-2.17		Estimated Solubility Method
log10ws	-2.27		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	1.249		Crippen Method
mcvol	178.590	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1967.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1950.00		NIST Webbook

rinpol	1950.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1973.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	1959.00		NIST Webbook
rinpol	1946.00		NIST Webbook
tb	822.67	K	Joback Method
tc	1107.17	K	Joback Method
tf	445.90	K	Aqueous Solubility Prediction Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.24	J/mol×K	822.67	Joback Method
cpg	587.91	J/mol×K	870.09	Joback Method
cpg	606.18	J/mol×K	917.50	Joback Method
cpg	623.09	J/mol×K	964.92	Joback Method
cpg	638.65	J/mol×K	1012.34	Joback Method
cpg	652.92	J/mol×K	1059.75	Joback Method
cpg	665.92	J/mol×K	1107.17	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52313&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume