Pentobarbital

Other names:	(.+/-.))-Pentobarbital
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylbutyl)-
	5-Ethyl-5-(1-methylbutyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Ethyl-5-(1-methylbutyl)barbituric acid
	5-Ethyl-5-(1-methylbutyl)barbituric acidcid
	5-Ethyl-5-(1-methylbutyl)malonylurea
	5-Ethyl-5-(sec-pentyl)barbituric acid
	Barbituric acid, 5-ethyl-5-(1-methylbutyl)-
	Dorsital
	Ethaminal
	Ethyl-propylmethylcarbinylbarbituric acid
	Mebubarbital
	Mebumal
	NSC 28708
	Nebralin
	Nembutal
	Neodorm
	Neodorm (new)
	Pentabarbital
	Pentabarbitone
	Pentobarbitone
	Pentobarbiturate
	Pentobarbituric acid
	Phetobarbitone
	Rivadorm
	component of Emesert
	component of Synirin
Inchi:	InChI=1S/C11H18N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(
InchiKey:	WEXRUCMBJFQVBZ-UHFFFAOYSA-N
Formula:	C11H18N2O3
SMILES:	CCCC(C)C1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	226.27
CAS:	76-74-4

Physical Properties

Property code	Value	Unit	Source

gf	-134.09	kJ/mol	Joback Method
hf	-543.57	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	65.23	kJ/mol	Joback Method
log10ws	-2.51		Aqueous Solubility Prediction Method
log10ws	-2.39		Estimated Solubility Method
logp	1.185		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1779.70		NIST Webbook
rinpol	293.65		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1779.70		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1750.00		NIST Webbook

rinpol	1719.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	293.65		NIST Webbook
rinpol	295.45		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1711.50		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	770.99	K	Joback Method
tc	1023.28	K	Joback Method
tf	403.00 ± 4.00	K	NIST Webbook
tf	402.77	K	Aqueous Solubility Prediction Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.25	J/mol×K	770.99	Joback Method
cpg	568.87	J/mol×K	813.04	Joback Method
cpg	586.48	J/mol×K	855.09	Joback Method
cpg	603.10	J/mol×K	897.13	Joback Method
cpg	618.72	J/mol×K	939.18	Joback Method
cpg	633.37	J/mol×K	981.23	Joback Method
cpg	647.06	J/mol×K	1023.28	Joback Method

Sources

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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76744&Units=SI

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