5-ETHYL-5-(1-METHYLBUTYL)-2,4,6(1H,3H,5H)-PY

Other names: (.+/-.))-Pentobarbital
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylbutyl)-
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
pentobarbital

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]: 226.28

Physical Properties

Property code	Value	Unit	Source
hfus	23.97	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
rinpol	1716.00		NIST Webbook
rinpol	293.65		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1779.70		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1779.70		NIST Webbook
rinpol	1733.00		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	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	1740.00		NIST Webbook
rinpol	1711.50		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1763.00		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	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	1719.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tf	402.77	K	Aqueous Solubility Prediction Method
tf	403.00 ± 4.00	K	NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76744&Units=SI

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

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point