Amobarbital

Other names:

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methylbutyl)-
5-Ethyl-5-(3-methylbutyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Ethyl-5-(3-methylbutyl)barbituric acid
5-Ethyl-5-isoamylbarbituric acid
5-Ethyl-5-isoamylmalonyl urea
5-Ethyl-5-isopentylbarbituric acid
5-Isoamyl-5-ethylbarbituric acid
Amal
Amasust
Amital
Amobarbitone
Amospan
Amybal
Amylbarbitone
Amylobarbital
Amylobarbitone
Amytal
Barbamil
Barbamyl
Barbamyl acid
Barbituric acid, 5-ethyl-5-isoamyl-
Barbituric acid, 5-ethyl-5-isopentyl-
Binoctal
Dorlotyn
Dormytal
Ethylisopentylbarbituric acid
Eunoctal
Isoamylethylbarbituric acid
Isomyl
Isomytal
Mylodorm
NSC 10815
Pentymal
Pentymalum
Robarb
Schiwanox
Sednotic
Somnal
Stadadorm
Sumital

	Talamo
Inchi:	InChI=1S/C11H18N2O3/c1-4-11(6-5-7(2)3)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(
InchiKey:	VIROVYVQCGLCII-UHFFFAOYSA-N
Formula:	C11H18N2O3
SMILES:	CCC1(CCC(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	226.27
CAS:	57-43-2

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	-2.64		Aqueous Solubility Prediction Method
log10ws	-2.47		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.47		Estimated Solubility Method
logp	1.185		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1705.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1696.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1752.90		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1690.00		NIST Webbook

rinpol	1737.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1720.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1714.00	NIST Webbook
rinpol	1702.00	NIST Webbook
rinpol	1715.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1695.00	NIST Webbook
rinpol	1685.00	NIST Webbook
rinpol	1692.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1690.00	NIST Webbook
rinpol	1694.00	NIST Webbook
rinpol	1718.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1710.00	NIST Webbook
rinpol	1711.00	NIST Webbook
rinpol	1712.00	NIST Webbook
rinpol	1713.00	NIST Webbook
rinpol	1721.00	NIST Webbook
rinpol	1718.00	NIST Webbook
rinpol	1689.00	NIST Webbook
rinpol	1692.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1691.00	NIST Webbook
rinpol	1691.00	NIST Webbook
rinpol	1695.00	NIST Webbook
rinpol	1703.00	NIST Webbook
rinpol	1697.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1718.00	NIST Webbook
rinpol	1714.00	NIST Webbook
rinpol	1725.00	NIST Webbook
rinpol	1752.90	NIST Webbook
rinpol	1737.00	NIST Webbook
rinpol	1689.00	NIST Webbook
rinpol	1695.00	NIST Webbook
rinpol	1714.00	NIST Webbook
rinpol	1750.00	NIST Webbook
rinpol	1712.00	NIST Webbook
rinpol	1735.00	NIST Webbook
rinpol	1700.00	NIST Webbook

rinpol	1695.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1715.00		NIST Webbook
tb	770.99	K	Joback Method
tc	1023.28	K	Joback Method
tf	433.00 ± 1.00	K	NIST Webbook
tf	429.75	K	Aqueous Solubility Prediction Method
tf	426.00 ± 4.00	K	NIST Webbook
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57432&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
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

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