Thiopental

Other names: (.+/-.)-Thiopental
2-Thio-5-ethyl-5-sec-pentylbarbituric acid
4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(1-methylbutyl)-2-thioxo-
5-Ethyl-5-(1-methylbutyl)-2-thiobarbituric acid
5-Ethyl-5-(1-methylbutyl)-2-thioxodihydro-4,6(1H,5H)-pyrimidinedione
71-73-8
7438-31-5
Barbituric acid, 5-ethyl-5-(1-methylbutyl)-2-thio-
Intraval
Penthiobarbital
Pentothiobarbital
Thiomebumal
Thionembutal
Thiopentobarbital
Thiopentobarbitone
Thiopentobarbituric acid
Thiopentone
Thiothal
Tiopentale

Inchi: InChI=1S/C11H18N2O2S/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3

InchiKey: IUJDSEJGGMCXSG-UHFFFAOYSA-N

Formula: C11H18N2O2S

SMILES: CCCC(C)C1(CC)C(=O)NC(=S)NC1=O

Mol. weight [g/mol]: 242.34

CAS: 76-75-5

Physical Properties

Property code	Value	Unit	Source
gf	79.35	kJ/mol	Joback Method
hf	-290.77	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-3.36		Estimated Solubility Method
log10ws	-3.36		Aqueous Solubility Prediction Method
logp	1.350		Crippen Method

mcvol	190.140	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1842.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1859.00		NIST Webbook
tb	775.81	K	Joback Method
tc	1031.19	K	Joback Method
tf	431.00 ± 1.00	K	NIST Webbook
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.33	J/mol×K	775.81	Joback Method
cpg	565.62	J/mol×K	818.37	Joback Method
cpg	582.17	J/mol×K	860.94	Joback Method
cpg	598.08	J/mol×K	903.50	Joback Method
cpg	613.44	J/mol×K	946.07	Joback Method
cpg	628.33	J/mol×K	988.63	Joback Method
cpg	642.85	J/mol×K	1031.19	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=C76755&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