Thiamylal

Other names:	4,6(1H,5H)-Pyrimidinedione, dihydro-5-(1-methylbutyl)-5-(2-propenyl)-2-thioxo-
	5-Allyl-5-(1-methylbutyl)-2-thiobarbituric acid
	Barbituric acid, 5-allyl-5-(1-methylbutyl)-2-thio-
	Surital
	Thioseconal
Inchi:	InChI=1S/C12H18N2O2S/c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h5,8H,2,4,6-7
InchiKey:	XLOMZPUITCYLMJ-UHFFFAOYSA-N
Formula:	C12H18N2O2S
SMILES:	C=CCC1(C(C)CCC)C(=O)NC(=S)NC1=O
Mol. weight [g/mol]:	254.35
CAS:	77-27-0

Physical Properties

Property code	Value	Unit	Source
gf	175.61	kJ/mol	Joback Method
hf	-185.98	kJ/mol	Joback Method
hfus	31.80	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-3.46		Estimated Solubility Method
log10ws	-3.46		Aqueous Solubility Prediction Method
logp	1.516		Crippen Method
mcvol	199.930	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
rinpol	1899.00		NIST Webbook
rinpol	1886.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	795.37	K	Joback Method
tc	1050.18	K	Joback Method
tf	405.65	K	Aqueous Solubility Prediction Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.95	J/mol×K	795.37	Joback Method
cpg	595.16	J/mol×K	837.84	Joback Method
cpg	611.67	J/mol×K	880.31	Joback Method
cpg	627.58	J/mol×K	922.77	Joback Method
cpg	643.00	J/mol×K	965.24	Joback Method
cpg	658.03	J/mol×K	1007.71	Joback Method
cpg	672.76	J/mol×K	1050.18	Joback Method

Sources

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=C77270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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