Talbutal

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylpropyl)-5-(2-propenyl)-
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methypropyl)-5-(2-propenyl)-
	5-(1-Methylpropyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Allyl-5-(1-methylpropyl) barbituric acid
	5-Allyl-5-sec-butyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Allyl-5-sec-butylbarbituric acid
	Barbituric acid, 5-allyl-5-sec-butyl-
	Butalbital
	Latusate
	Lotusate
	Profundol
	WIN 5095
	sec-Butyl allyl barbituric acid
Inchi:	InChI=1S/C11H16N2O3/c1-4-6-11(7(3)5-2)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3
InchiKey:	BJVVMKUXKQHWJK-UHFFFAOYSA-N
Formula:	C11H16N2O3
SMILES:	C=CCC1(C(C)CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	224.26
CAS:	115-44-6

Physical Properties

Property code	Value	Unit	Source
gf	-46.25	kJ/mol	Joback Method
hf	-418.14	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-2.02		Estimated Solubility Method
log10ws	-2.02		Aqueous Solubility Prediction Method
logp	0.961		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1701.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1704.00		NIST Webbook

rinpol	1677.00		NIST Webbook
tb	767.67	K	Joback Method
tc	1025.00	K	Joback Method
tf	642.97	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.76	J/mol×K	767.67	Joback Method
cpg	542.80	J/mol×K	810.56	Joback Method
cpg	559.87	J/mol×K	853.45	Joback Method
cpg	575.99	J/mol×K	896.34	Joback Method
cpg	591.16	J/mol×K	939.22	Joback Method
cpg	605.41	J/mol×K	982.11	Joback Method
cpg	618.77	J/mol×K	1025.00	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=C115446&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