Probarbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylethyl)-
	5-Ethyl-5-(1-methylethyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Ethyl-5-isopropylbarbituric acid
	Barbituric acid, 5-ethyl-5-isopropyl-
	Ethylisopropylbarbituric acid
	Ipral
	Irenal
	Isopropyl ethyl barbituric acid
	NSC 120742
	Probarbitone
	Vasalgin
Inchi:	InChI=1S/C9H14N2O3/c1-4-9(5(2)3)6(12)10-8(14)11-7(9)13/h5H,4H2,1-3H3,(H2,10,11,1
InchiKey:	HHLXJTDUHFBYAU-UHFFFAOYSA-N
Formula:	C9H14N2O3
SMILES:	CCC1(C(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	198.22
CAS:	76-76-6

Physical Properties

Property code	Value	Unit	Source
gf	-150.93	kJ/mol	Joback Method
hf	-502.29	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.21		Estimated Solubility Method
log10ws	-2.21		Aqueous Solubility Prediction Method
logp	0.405		Crippen Method
mcvol	151.480	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	725.23	K	Joback Method
tc	989.41	K	Joback Method
tf	474.48	K	Aqueous Solubility Prediction Method

vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.01	J/mol×K	725.23	Joback Method
cpg	458.67	J/mol×K	769.26	Joback Method
cpg	475.43	J/mol×K	813.29	Joback Method
cpg	491.29	J/mol×K	857.32	Joback Method
cpg	506.23	J/mol×K	901.35	Joback Method
cpg	520.27	J/mol×K	945.38	Joback Method
cpg	533.40	J/mol×K	989.41	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=C76766&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