Barbituric acid, 5-propyl-5-(2-methylpropyl)

Inchi: InChI=1S/C11H18N2O3/c1-4-5-11(6-7(2)3)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3,(
InchiKey: JKOZKFJTOIXANY-UHFFFAOYSA-N
Formula: C11H18N2O3
SMILES: CCCC1(CC(C)C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 226.27

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	-2.52		Crippen Method
logp	1.185		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1693.00		NIST Webbook
rinpol	1693.00		NIST Webbook
tb	770.99	K	Joback Method
tc	1023.28	K	Joback Method
tf	644.73	K	Joback Method
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=R17480&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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