Barbituric acid, 5-ethyl-5-(3-hydroxyisopentyl)-

Other names:	5-Aethyl-5-(3-hydroxyisoamyl)barbitursaeure
	5-Ethyl-5-(3-hydroxyisopentyl)barbituric acid
	Faktor I
	3'-Hydroxyamobarbital
Inchi:	InChI=1S/C11H18N2O4/c1-4-11(6-5-10(2,3)17)7(14)12-9(16)13-8(11)15/h17H,4-6H2,1-3
InchiKey:	PUVZPWLDMBLALZ-UHFFFAOYSA-N
Formula:	C11H18N2O4
SMILES:	CCC1(CCC(C)(C)O)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	242.27
CAS:	1421-07-4

Physical Properties

Property code	Value	Unit	Source
gf	-265.63	kJ/mol	Joback Method
hf	-699.27	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	81.00	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	0.300		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	860.38	K	Joback Method
tc	1100.62	K	Joback Method
tf	722.97	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.58	J/mol×K	860.38	Joback Method
cpg	624.10	J/mol×K	900.42	Joback Method
cpg	638.79	J/mol×K	940.46	Joback Method
cpg	652.70	J/mol×K	980.50	Joback Method
cpg	665.87	J/mol×K	1020.54	Joback Method

cpg	678.34	J/mol×K	1060.58	Joback Method
cpg	690.15	J/mol×K	1100.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1421074&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume