5-Ethyl-5(1-ethylpropyl) 2-thiobarbituric acid

Inchi: InChI=1S/C11H18N2O2S/c1-4-7(5-2)11(6-3)8(14)12-10(16)13-9(11)15/h7H,4-6H2,1-3H3
InchiKey: VMBXKUPZOMUHQT-UHFFFAOYSA-N
Formula: C11H18N2O2S
SMILES: CCC(CC)C1(CC)C(=O)NC(=S)NC1=O
Mol. weight [g/mol]: 242.34
CAS: 87171-21-9

Physical Properties

Property code	Value	Unit	Source
gf	79.35	kJ/mol	Joback Method
hf	-290.77	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	1.350		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	775.81	K	Joback Method
tc	1031.19	K	Joback Method
tf	640.18	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.33	J/mol×K	775.81	Joback Method
cpg	565.62	J/mol×K	818.37	Joback Method
cpg	582.17	J/mol×K	860.94	Joback Method
cpg	598.08	J/mol×K	903.50	Joback Method
cpg	613.44	J/mol×K	946.07	Joback Method
cpg	628.33	J/mol×K	988.63	Joback Method
cpg	642.85	J/mol×K	1031.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87171219&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume