Barbituric acid, 5-hydroxy-5-thiosemicarbazido-

Inchi: InChI=1S/C5H7N5O4S/c6-3(15)9-10-5(14)1(11)7-4(13)8-2(5)12/h10,14H,(H3,6,9,15)(H2

InchiKey: GOHDTOFXBVDEDM-UHFFFAOYSA-N

Formula: C5H7N5O4S

SMILES: NC(=S)NNC1(O)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 233.21

Physical Properties

Property code	Value	Unit	Source
gf	43.30	kJ/mol	Joback Method
hf	-279.45	kJ/mol	Joback Method
hfus	36.04	kJ/mol	Joback Method
hvap	99.18	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	-3.621		Crippen Method
mcvol	142.980	ml/mol	McGowan Method
pc	9499.60	kPa	Joback Method
tb	969.24	K	Joback Method
tc	1239.16	K	Joback Method
tf	875.78	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.58	J/mol×K	969.24	Joback Method
cpg	456.14	J/mol×K	1014.23	Joback Method
cpg	466.33	J/mol×K	1059.21	Joback Method
cpg	476.22	J/mol×K	1104.20	Joback Method
cpg	485.86	J/mol×K	1149.19	Joback Method
cpg	495.31	J/mol×K	1194.18	Joback Method
cpg	504.61	J/mol×K	1239.16	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=B6008719&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