5,5-Dibromobarbituric acid

Inchi: InChI=1S/C4H2Br2N2O3/c5-4(6)1(9)7-3(11)8-2(4)10/h(H2,7,8,9,10,11)
InchiKey: AMATXUCYHHHHHB-UHFFFAOYSA-N
Formula: C4H2Br2N2O3
SMILES: O=C1NC(=O)C(Br)(Br)C(=O)N1
Mol. weight [g/mol]: 285.88
CAS: 511-67-1

Physical Properties

Property code	Value	Unit	Source
gf	-161.95	kJ/mol	Joback Method
hf	-341.15	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	-0.162		Crippen Method
mcvol	116.030	ml/mol	McGowan Method
pc	8916.78	kPa	Joback Method
tb	743.59	K	Joback Method
tc	1060.96	K	Joback Method
tf	700.44	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.26	J/mol×K	743.59	Joback Method
cpg	258.17	J/mol×K	796.48	Joback Method
cpg	268.64	J/mol×K	849.38	Joback Method
cpg	278.67	J/mol×K	902.27	Joback Method
cpg	288.27	J/mol×K	955.17	Joback Method
cpg	297.44	J/mol×K	1008.06	Joback Method
cpg	306.20	J/mol×K	1060.96	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=C511671&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