Barbituric acid, 5-nitro-

Other names: 5-nitrobarbituric acid
Inchi: InChI=1S/C4H3N3O5/c8-2-1(7(11)12)3(9)6-4(10)5-2/h1H,(H2,5,6,8,9,10)
InchiKey: ABICJYZKIYUWEE-UHFFFAOYSA-N
Formula: C4H3N3O5
SMILES: O=C1NC(=O)C([N+](=O)[O-])C(=O)N1
Mol. weight [g/mol]: 173.08
CAS: 28176-10-5

Physical Properties

Property code	Value	Unit	Source
gf	-149.55	kJ/mol	Joback Method
hf	-419.81	kJ/mol	Joback Method
hfs	-679.90	kJ/mol	NIST Webbook
hfus	27.02	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-2.28		Aqueous Solubility Prediction Method
logp	-2.002		Crippen Method
mcvol	98.450	ml/mol	McGowan Method
pc	6609.82	kPa	Joback Method
tb	762.87	K	Joback Method
tc	1063.49	K	Joback Method
tf	453.65	K	Aqueous Solubility Prediction Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.87	J/mol×K	762.87	Joback Method
cpg	290.39	J/mol×K	812.97	Joback Method
cpg	300.26	J/mol×K	863.08	Joback Method
cpg	308.24	J/mol×K	913.18	Joback Method
cpg	314.07	J/mol×K	963.28	Joback Method

cpg	317.49	J/mol×K	1013.38	Joback Method
cpg	318.25	J/mol×K	1063.49	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28176105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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