Uroxine

Other names:	5,5'-Bibarbituric acid, 5,5'-dihydroxy- 5,5'-Dihydroxy-5,5'-dibarbituric acid 5,5'-dihydroxy-5,5'-bipyrimidinehexaone Alloxantin Alloxantin, dihydrate Uroxin [5,5'-Bipyrimidine]-2,2',4,4',6,6'(1H,1'H,3H,3'H,5H,5'H)-hexone, 5,5'-dihydroxy- alloxanthin
Inchi:	InChI=1S/C8H6N4O8/c13-1-7(19,2(14)10-5(17)9-1)8(20)3(15)11-6(18)12-4(8)16/h19-20H
InchiKey:	IWDDXZKCDHOOSF-UHFFFAOYSA-N
Formula:	C8H6N4O8
SMILES:	O=C1NC(=O)C(O)(C2(O)C(=O)NC(=O)NC2=O)C(=O)N1
Mol. weight [g/mol]:	286.16
CAS:	76-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-603.94	kJ/mol	Joback Method
hf	-1048.75	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	117.83	kJ/mol	Joback Method
log10ws	-1.99		Estimated Solubility Method
log10ws	-1.99		Aqueous Solubility Prediction Method
logp	-4.819		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
pc	10161.94	kPa	Joback Method
tb	1207.50	K	Joback Method
tc	1497.96	K	Joback Method
tf	1193.56	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.77	J/mol×K	1207.50	Joback Method
cpg	641.46	J/mol×K	1255.91	Joback Method
cpg	649.59	J/mol×K	1304.32	Joback Method
cpg	656.09	J/mol×K	1352.73	Joback Method
cpg	660.89	J/mol×K	1401.14	Joback Method
cpg	663.93	J/mol×K	1449.55	Joback Method
cpg	665.16	J/mol×K	1497.96	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
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76244&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
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

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