ALLOXANTIN

Other names:	5,5'-Bibarbituric acid, 5,5'-dihydroxy- 5,5'-Dihydroxy-5,5'-dibarbituric acid 5,5'-dihydroxy-5,5'-bipyrimidinehexaone 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

Physical Properties

Property code	Value	Unit	Source
hfus	31.15	kJ/mol	Joback Method
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-1.99		Aqueous Solubility Prediction Method
log10ws	-1.99		Estimated Solubility Method
logp	-4.819		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
tf	536.95	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76244&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point