Xanthine

Other names:	1H-Purine-2,6-diol
	1H-Purine-2,6-dione, 3,7-dihydro-
	2,6(1,3)-Purinedion
	2,6-Dihydroxypurine
	2,6-Dioxo-1,2,3,6-tetrahydropurine
	2,6-Dioxopurine
	3,7-Dihydro-1H-purine-2,6-dione
	3,7-dihydropurine-2,6-dione
	9H-Purine-2,6(1H,3H)-dione
	9H-Purine-2,6-diol
	Isoxanthine
	NSC 14664
	Pseudoxanthine
	Purine-2,6(1H,3H)-dione
	Purine-2,6-diol
	USAF CB-17
	Xan
	Xanthic oxide
	Xanthin
	purine-2(3H),6(1H)-dione
	purine-2,6-dione, 3,7-dihydro-
Inchi:	InChI=1S/C5H4N4O2/c10-4-2-3(7-1-6-2)8-5(11)9-4/h1H,(H3,6,7,8,9,10,11)
InchiKey:	LRFVTYWOQMYALW-UHFFFAOYSA-N
Formula:	C5H4N4O2
SMILES:	Oc1nc(O)c2nc[nH]c2n1
Mol. weight [g/mol]:	152.11
CAS:	69-89-6

Physical Properties

Property code	Value	Unit	Source
chs	-2159.70 ± 0.88	kJ/mol	NIST Webbook
hfs	-379.60 ± 0.92	kJ/mol	NIST Webbook
ie	8.55	eV	NIST Webbook
ie	9.30 ± 0.20	eV	NIST Webbook
ie	8.89 ± 0.03	eV	NIST Webbook
log10ws	-3.87		Aqueous Solubility Prediction Method

logp	-0.718		Crippen Method
mcvol	94.050	ml/mol	McGowan Method
ss	161.10	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	151.34	J/mol×K	298.50	NIST Webbook
hvapt	172.40	kJ/mol	421.00	Thermochemical Properties of Xanthine and Hypoxanthine Revisited

Sources

Saturation molalities and standard molar enthalpies of solution of cytosine(cr), hypoxanthine(cr), and xanthine(cr) in H2O(l):	https://www.doi.org/10.1016/j.jct.2004.04.005
Thermochemical Properties of Xanthine and Hypoxanthine Revisited:	https://www.doi.org/10.1021/acs.jced.7b00085
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=C69896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions

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