1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-

Other names:	1H-Purine-2,6,8-triol
	2,6,8-Trihydroxypurine
	2,6,8-Trioxopurine
	2,6,8-Trioxypurine
	7,9-Dihydro-1H-purine-2,6,8(3H)-trione
	8-Hydroxyxanthine
	Lithic acid
	NSC 3975
	Purine-2,6,8(1H,3H,9H)-trione
	Purine-2,6,8-triol
	Purine-3,6,8(1H,3H,9H)-trione
	uric acid
Inchi:	InChI=1S/C5H4N4O3/c10-3-1-2(7-4(11)6-1)8-5(12)9-3/h(H4,6,7,8,9,10,11,12)
InchiKey:	LEHOTFFKMJEONL-UHFFFAOYSA-N
Formula:	C5H4N4O3
SMILES:	O=c1[nH]c(=O)c2[nH]c(=O)[nH]c2[nH]1
Mol. weight [g/mol]:	168.11

Physical Properties

Property code	Value	Unit	Source
chs	-1920.40 ± 0.84	kJ/mol	NIST Webbook
chs	-1924.50	kJ/mol	NIST Webbook
hfs	-618.81 ± 0.88	kJ/mol	NIST Webbook
ie	8.15	eV	NIST Webbook
log10ws	-3.70		Aqueous Solubility Prediction Method
log10ws	-3.93		Estimated Solubility Method
logp	-3.695		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
ss	173.20	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cps	166.15	J/mol×K	297.10	NIST Webbook

Sources

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=C69932&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
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