6H-Purin-6-one, 1,7-dihydro-

Other names:	1,7-Dihydro-6H-purine-6-one
	1,7-dihydro-6H-purin-6-one
	3H-Purin-6-ol
	6(1H)-Purinone
	6-Hydroxy-1H-purine
	6-Oxopurine
	6-hydroxypurine
	6H-Purin-6-one, 1,9-dihydro-
	9H-Purin-6(1H)-one
	9H-Purin-6-ol
	HX
	Hypoxanthine enol
	NSC 14665
	Purin-6-ol
	Purine-6-ol
	Sarcine
	Sarkin
	Sarkine
	hypoxanthine
	purin-6(1H)-one
	purin-6(3H)-one
Inchi:	InChI=1S/C5H4N4O/c10-5-3-4(7-1-6-3)8-2-9-5/h1-2H,(H2,6,7,8,9,10)
InchiKey:	FDGQSTZJBFJUBT-UHFFFAOYSA-N
Formula:	C5H4N4O
SMILES:	Oc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	136.11
CAS:	68-94-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	-0.423		Crippen Method
mcvol	88.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	160.30	kJ/mol	411.00	Thermochemical Properties of Xanthine and Hypoxanthine Revisited
rhos	1600.00	kg/m3	298.15	Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(cr), and xanthine(cr) in H2O(l)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Saturation molalities and standard molar enthalpies of solution of cytidine(cr), hypoxanthine(cr), thymidine(cr), thymine(cr), uridine(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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhos:	Solid Density

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.