6-Azathymine

Other names:	1,2,4-Triazine-3,5(2H,4H)-dione, 6-methyl-
	3,5-Dihydroxy-6-methyl-1,2,4-triazine
	5-methyl-6-azauracil
	6-Methyl-1,2,4-triazine-3,5-dione
	6-Methyl-as-triazine-3,5(2H,4H)-dione
	6-methyl-1,2,4-triazine-3,5(2H,4H)-dione
	6-methyl-1,2,4-triazine-3,5-diol
	NSC 3426
	NSC 38620
	USAF CB-28
	as-Triazine-3,5(2H,4H)-dione, 6-methyl-
	as-Triazine-3,5-diol, 6-methyl-
Inchi:	InChI=1S/C4H5N3O2/c1-2-3(8)5-4(9)7-6-2/h1H3,(H2,5,7,8,9)
InchiKey:	XZWMZFQOHTWGQE-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	Cc1n[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	127.10
CAS:	932-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.00		Crippen Method
logp	-2.197		Crippen Method
mcvol	85.140	ml/mol	McGowan Method
rinpol	1380.70		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	112.50 ± 2.30	kJ/mol	380.50	NIST Webbook

hvapt	109.10	kJ/mol	298.15	Experimental and computational thermochemical studies of 6-azauracil derivatives

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemical studies of 6-azauracil derivatives:	https://www.doi.org/10.1016/j.jct.2015.12.020
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C932536&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices