6-Aza-2-thiothymine

Other names:	1,2,4-Triazin-5(2H)-one, 3,4-dihydro-6-methyl-3-thioxo- 2-thio-6-azathymine 3-mercapto-6-methyl-1,2,4-triazin-5(2H)-one 6-Azathiothymine 6-Methyl-3-thioxo-5-oxo-2,3,4,5-tetrahydro-1,2,4-triazine 6-methyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2H)-one as-Triazin-5-ol, 3-mercapto-6-methyl- as-Triazine-3,5(2H,4H)-dione, 6-methyl-3-thio-
Inchi:	InChI=1S/C4H5N3OS/c1-2-3(8)5-4(9)7-6-2/h1H3,(H2,5,7,8,9)
InchiKey:	NKOPQOSBROLOFP-UHFFFAOYSA-N
Formula:	C4H5N3OS
SMILES:	Cc1n[nH]c(=S)[nH]c1=O
Mol. weight [g/mol]:	143.17
CAS:	615-76-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.42		Crippen Method
logp	-0.828		Crippen Method
mcvol	95.620	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	120.10	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=C615769&Units=SI

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