2-Thiouracil

Other names:	2,3-Dihydro-2-thioxo-4(1H)-pyrimidinone
	2-Mercapto-4-hydroxypyrimidine
	2-Mercapto-4-pyrimidinol
	2-Mercapto-4-pyrimidone
	2-Mercaptopyrimid-4-one
	2-TU
	2-Thio-1,3-pyrimidin-4-one
	4(1H)-Pyrimidinone, 2,3-dihydro-2-thioxo-
	4-Hydroxy-2-mercaptopyrimidine
	4-Hydroxy-2-pyrimidinethiol
	4-Pyrimidinol, 2-mercapto-
	6-Hydroxy-2-mercaptopyrimidine
	6-Thiouracil
	Antagothyroid
	Antagothyroil
	Deracil
	NSC 19473
	Nobilen
	TU
	Thiouracil
	Uracil, 2-thio-
Inchi:	InChI=1S/C4H4N2OS/c7-3-1-2-5-4(8)6-3/h1-2H,(H2,5,6,7,8)
InchiKey:	ZEMGGZBWXRYJHK-UHFFFAOYSA-N
Formula:	C4H4N2OS
SMILES:	O=c1cc[nH]c(=S)[nH]1
Mol. weight [g/mol]:	128.15
CAS:	141-90-2

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-2.26		Aqueous Solubility Prediction Method
logp	-0.531		Crippen Method
mcvol	85.640	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C141902&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume