4(1H)-Pyrimidinone, 6-amino-2,3-dihydro-2-thioxo-

Other names:	AB 48
	Uracil, 6-amino-2-thio-
	2-Mercapto-6-aminouracil
	2-Thio-6-aminouracil
	4-Amino-2-thiouracil
	6-Amino-2-thiouracil
	6-Amino-4-keto-2-thiopyrimidine
	6-Aminothiouracil
	NSC 1587
	NSC 202018
	6-amino-2-thiouracil hydrate
Inchi:	InChI=1S/C4H5N3OS/c5-2-1-3(8)7-4(9)6-2/h1H,(H4,5,6,7,8,9)
InchiKey:	YFYYRKDBDBILSD-UHFFFAOYSA-N
Formula:	C4H5N3OS
SMILES:	Nc1cc(=O)[nH]c(=S)[nH]1
Mol. weight [g/mol]:	143.17
CAS:	1004-40-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.18		Crippen Method
logp	-0.949		Crippen Method
mcvol	95.620	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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