

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:	YFYRKDBDBILSD-UHFFFAOYSA-N
Formula:	C4H5N3OS
SMILES:	<chem>Nc1cc(=O)[nH]c(=S)[nH]1</chem>
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/ci9903071
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

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