4-AMINO-6-HYDROXY-2-MERCAPTOPYRIMIDINE MONOHYDRATE

Other names: AB-18
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

Physical Properties

Property code	Value	Unit	Source
ie	7.74	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	-0.949		Crippen Method
mcvol	95.620	ml/mol	McGowan Method
tf	540.51	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004406&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point