

6-Thioxanthine

Other names:	2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo- 2-Hydroxy-6-mercaptopurine 2-Hydroxy-6-thiopurine 3,6-Dihydro-6-thioxo-9H-purine-2(1H)-one 6-Mercaptioxanthine Xanthine, 6-thio- Imidazolo[4, 5-d]pyrimidin-6(5H)-one, 4, 7-dihydro-4-thione- 6-Thioxo-1,3,6,7-tetrahydro-purin-2-one Purin-2-ol, 6-mercapto (keto form) NSC 12160
Inchi:	InChI=1S/C5H4N4OS/c10-5-8-3-2(4(11)9-5)6-1-7-3/h1H,(H3,6,7,8,9,10,11)
InchiKey:	RJOXFJDOUQJOMQ-UHFFFAOYSA-N
Formula:	C5H4N4OS
SMILES:	O=c1[nH]c(=S)c2nc[nH]c2[nH]1
Mol. weight [g/mol]:	168.18
CAS:	2002-59-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.97		Crippen Method
logp	-1.137		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2002597&Units=SI

Legend

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

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