

6-THIOXANTHINE

Other names:	2-Hydroxy-6-mercaptopurine
	2-Hydroxy-6-thiopurine
	2H-Purin-2-one, 1,3,6,7-tetrahydro-6-thioxo-
	3,6-Dihydro-6-thioxo-9H-purine-2(1H)-one
	6-Mercaptoxanthine
	6-Thioxo-1,3,6,7-tetrahydro-purin-2-one
	Imidazolo[4, 5-d]pyrimidin-6(5H)-one, 4, 7-dihydro-4-thione-
	NSC 12160
	Purin-2-ol, 6-mercapto (keto form)
	Xanthine, 6-thio-
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

Physical Properties

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

Sources

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=C2002597&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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