2-MERCAPTO-6-PURINOL

Other names:	6H-Purin-6-one, 1,2,3,7-tetrahydro-2-thioxo- Xanthine, 2-thio- 2-Mercapto-6-hydroxypurine 2-Thioxanthine 6-Hydroxypurine-2-thiol 1,2,3,7-Tetrahydro-2-thioxo-6H-purin-6-one 2-Thio-6-oxypurine Hypoxanthine, 2-mercapto- 2-Mercaptohypoxanthine 6H-Purin-6-one, 1,2,3,9-tetrahydro-2-thioxo- NSC 36822 NSC 680828
Inchi:	InChI=1S/C5H4N4OS/c10-4-2-3(7-1-6-2)8-5(11)9-4/h1H,(H3,6,7,8,9,10,11)
InchiKey:	XNHFAGRBSMMFKL-UHFFFAOYSA-N
Formula:	C5H4N4OS
SMILES:	Oc1nc(S)nc2[nH]cnc12
Mol. weight [g/mol]:	168.18

Physical Properties

Property code	Value	Unit	Source
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-3.49		Cheméo Relay (1.0)
logp	-0.135		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2487403&Units=SI

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):

Legend

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