2(1H)-Pyrimidinethione, tetrahydro-1,3-dimethyl-

Other names: N,N'-Dimethyltrimethylenethiourea
Tetrahydro-1,3-dimethyl-2(1H)-pyrimidinethione
Inchi: InChI=1S/C6H12N2S/c1-7-4-3-5-8(2)6(7)9/h3-5H2,1-2H3
InchiKey: JILASYJQVXOLSP-UHFFFAOYSA-N
Formula: C6H12N2S
SMILES: CN1CCCN(C)C1=S
Mol. weight [g/mol]: 144.24
CAS: 16597-35-6

Physical Properties

Property code	Value	Unit	Source
ie	7.30	eV	NIST Webbook
ie	7.58	eV	NIST Webbook
log10ws	-0.72		Crippen Method
logp	0.539		Crippen Method
mcvol	116.550	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=C16597356&Units=SI

Legend

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

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