

5,6-Dihydro-5-methyl-4H-1,3,5-dithiazine

Other names:	4H-1,3,5-Dithiazine, dihydro-5-methyl-dihydro-5-methyl-4H-1,3,5-dithiazine
Inchi:	InChI=1S/C4H9NS2/c1-5-2-6-4-7-3-5/h2-4H2,1H3
InchiKey:	QMWSBGCIPZEDPP-UHFFFAOYSA-N
Formula:	C4H9NS2
SMILES:	CN1CSCSC1
Mol. weight [g/mol]:	135.25
CAS:	6302-94-9

Physical Properties

Property code	Value	Unit	Source
chs	-4035.30	kJ/mol	NIST Webbook
hfs	-22.80	kJ/mol	NIST Webbook
log10ws	-1.21		Crippen Method
logp	1.271		Crippen Method
mcvol	99.040	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6302949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
hfs:	Solid phase enthalpy of formation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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