

2(3H)-Benzothiazolethione, 3-methyl-

Other names:	2-Benzothiazolinethione, 3-methyl- N-Methylbenzothiazoline-2-thione 3-Methyl-1,3-benzothiazoline-2-thione 3-Methylbenzothiazole-2-thione 3-Methylbenzothiazoline-2-thione 3-Methylbenzo[d]thiazoline-2-thione N-Methylbenzothiazole-2-thione 3-Methyl-3H-benzothiazole-2-thione 3-methylbenzothiazole-2(3H)-thione
Inchi:	InChI=1S/C8H7NS2/c1-9-6-4-2-3-5-7(6)11-8(9)10/h2-5H,1H3
InchiKey:	IRNRNPZAKHEAW-UHFFFAOYSA-N
Formula:	C8H7NS2
SMILES:	Cn1c(=S)sc2ccccc21
Mol. weight [g/mol]:	181.28
CAS:	2254-94-6

Physical Properties

Property code	Value	Unit	Source
ie	7.81	eV	NIST Webbook
log10ws	-5.17		Crippen Method
logp	2.969		Crippen Method
mvol	127.340	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2254946&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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