

Isothiazole, 4-methyl-

Other names:	4-Methylisothiazole
Inchi:	InChI=1S/C4H5NS/c1-4-2-5-6-3-4/h2-3H,1H3
InchiKey:	YUTQRQJTFPEEPB-UHFFFAOYSA-N
Formula:	C4H5NS
SMILES:	Cc1cnsc1
Mol. weight [g/mol]:	99.15
CAS:	693-90-3

Physical Properties

Property code	Value	Unit	Source
ie	9.25	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.452		Crippen Method
mcvol	74.090	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=C693903&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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<https://www.chemeo.com/cid/26-548-5/Isothiazole-4-methyl.pdf>

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