

2-Mercapto-4,5-dimethylthiazole

Other names:	2(3H)-Thiazolethione, 4,5-dimethyl-4-[5-Dimethyl-2-thiazolethiol 4,5-dimethylthiazole-2(3H)-thione
Inchi:	InChI=1S/C5H7NS2/c1-3-4(2)8-5(7)6-3/h1-2H3,(H,6,7)
InchiKey:	KKHBRTFQIYIHEI-UHFFFAOYSA-N
Formula:	C5H7NS2
SMILES:	Cc1nc(S)sc1C
Mol. weight [g/mol]:	145.25
CAS:	5351-51-9

Physical Properties

Property code	Value	Unit	Source
ie	7.56 ± 0.03	eV	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.049		Crippen Method
mcvol	104.530	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5351519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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