

1,3,4-Thiadiazol-2-amine, 5-(methylthio)-

Other names:	1,3,4-Thiadiazole, 2-amino-5-(methylthio)- 2-Amino-5-methylmercapto-1,3,4-thiadiazole 2-Amino-5-(methylthio)-1,3,4-thiadiazole
Inchi:	InChI=1S/C3H5N3S2/c1-7-3-6-5-2(4)8-3/h1H3,(H2,4,5)
InchiKey:	PCLAZAJARAIGGD-UHFFFAOYSA-N
Formula:	C3H5N3S2
SMILES:	CSc1nnc(N)s1
Mol. weight [g/mol]:	147.22
CAS:	5319-77-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Crippen Method
logp	0.842		Crippen Method
mcvol	96.310	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=C5319777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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