

1,2,4-Thiadiazole, 5-amino-3-(methylthio)-

Other names:	5-Amino-3-(methylthio)-1,2,4-thiadiazole 3-Methylmercapto-5-amino-1,2,4-thiadiazole 1,2,4-Thiadiazol-5-amine, 3-(methylthio)- 3-(Methylthio)-1,2,4-thiadiazol-5-amine
Inchi:	InChI=1S/C3H5N3S2/c1-7-3-5-2(4)8-6-3/h1H3,(H2,4,5,6)
InchiKey:	HQKQSHMJHHADQB-UHFFFAOYSA-N
Formula:	C3H5N3S2
SMILES:	CSc1nsc(N)n1
Mol. weight [g/mol]:	147.22
CAS:	6913-13-9

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

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=C6913139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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