1,3,4-Thiadiazole-2(3H)-thione, 5-methyl-

Other names:	d2-1,3,4-Thiadiazoline-5-thione, 2-methyl-
	2-Mercapto-5-methyl-1,3,4-thiadiazole
	2-Methyl-1,3,4-thiadiazole-5-thiol
	2-Methyl-1,3,4-thiadiazoline-5-thione
	2-Methyl-5-mercapto-1,3,4-thiadiazole
	5-Methyl-1,3,4-thiadiazole-2-thiol
	5-methyl-1,3,4-thiadiazole-2(3H)-thione
Inchi:	InChI=1S/C3H4N2S2/c1-2-4-5-3(6)7-2/h1H3,(H,5,6)
InchiKey:	FPVUWZFFEGYCGB-UHFFFAOYSA-N
Formula:	C3H4N2S2
SMILES:	Cc1nnc(S)s1
Mol. weight [g/mol]:	132.21
CAS:	29490-19-5

Physical Properties

Property code	Value	Unit	Source
ie	8.33	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	1.135		Crippen Method
mcvol	86.330	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=C29490195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy

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

Latest version available from:
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