

3H-1,2,4-Triazole-3-thione,2,4-dihydro-2,4,5-trimethyl-

Other names:	2,4,5-Trimethyl-1,2,4-triazole-3-thione
Inchi:	InChI=1S/C5H9N3S/c1-4-6-8(3)5(9)7(4)2/h1-3H3
InchiKey:	PUMDJKUSQNDNQI-UHFFFAOYSA-N
Formula:	C5H9N3S
SMILES:	Cc1nn(C)c(=S)n1C
Mol. weight [g/mol]:	143.21
CAS:	37526-42-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	0.797		Crippen Method
mcvol	108.140	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=C37526424&Units=SI

Legend

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

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