

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

Other names: «delta»2-1,3,4-Thiadiazoline-5-thione, 2,4-dimethyl-
Inchi: InChI=1S/C4H6N2S2/c1-3-5-6(2)4(7)8-3/h1-2H3
InchiKey: SXGPSEUHDNWBQE-UHFFFAOYSA-N
Formula: C4H6N2S2
SMILES: Cc1nn(C)c(=S)s1
Mol. weight [g/mol]: 146.23
CAS: 7111-96-8

Physical Properties

Property code	Value	Unit	Source
ie	7.97	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	1.520		Crippen Method
mcvol	100.420	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7111968&Units=SI>
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>

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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