

5-Phenyl-1,2,3-thiadiazole

Other names:	1,2,3-Thiadiazole, 5-phenyl-
Inchi:	InChI=1S/C8H6N2S/c1-2-4-7(5-3-1)8-6-9-10-11-8/h1-6H
InchiKey:	MXTVVTVVBOYKCU-UHFFFAOYSA-N
Formula:	C8H6N2S
SMILES:	c1ccc(-c2cnns2)cc1
Mol. weight [g/mol]:	162.21
CAS:	18212-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.205		Crippen Method
mcvol	116.670	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=C18212298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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<https://www.chemeo.com/cid/33-772-8/5-Phenyl-1-2-3-thiadiazole.pdf>

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