

4-Thiazolecarbonitrile, 5-amino-2-methylsulfonyl-

Inchi:	InChI=1S/C5H5N3O2S2/c1-12(9,10)5-8-3(2-6)4(7)11-5/h7H2,1H3
InchiKey:	MYIDZAGZFHCYTC-UHFFFAOYSA-N
Formula:	C5H5N3O2S2
SMILES:	CS(=O)(=O)c1nc(C#N)c(N)s1
Mol. weight [g/mol]:	203.24
CAS:	116529-27-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.67		Crippen Method
logp	4.800e-04		Crippen Method
mcvol	127.630	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=C116529272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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