

2-Thiophenesulfonyl chloride

Other names:	2-Thienylsulfonyl chloride Thiophene-2-sulfonyl chloride thiophene-2-sulphonyl chloride
Inchi:	InChI=1S/C4H3ClO2S2/c5-9(6,7)4-2-1-3-8-4/h1-3H
InchiKey:	VNNLHYZDXIBHKZ-UHFFFAOYSA-N
Formula:	C4H3ClO2S2
SMILES:	O=S(=O)(Cl)c1cccs1
Mol. weight [g/mol]:	182.65
CAS:	16629-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	1.676		Crippen Method
mcvol	104.440	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C16629199&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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<https://www.chemeo.com/cid/53-255-0/2-Thiophenesulfonyl-chloride.pdf>

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