2,5-Dichlorothiophene-3-sulfonyl chloride

Other names:	2,5-Dichlorothiophene-3-sulphonyl chloride
Inchi:	InChI=1S/C4HCl3O2S2/c5-3-1-2(4(6)10-3)11(7,8)9/h1H
InchiKey:	JJKSHSHZJOWSEC-UHFFFAOYSA-N
Formula:	C4HCl3O2S2
SMILES:	O=S(=O)(Cl)c1cc(Cl)sc1Cl
Mol. weight [g/mol]:	251.54
CAS:	56946-83-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Crippen Method
logp	2.982		Crippen Method
mcvol	128.920	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=C56946839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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