

2,5-Dichlorothiophene-3-sulphonyl 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

Physical Properties

Property code	Value	Unit	Source
logp	2.982		Crippen Method
mcvol	128.920	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56946839&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/20-108-9/2-5-Dichlorothiophene-3-sulphonyl-chloride.pdf>

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