3-(2,6-Dichlorophenyl)-5-methylisoxazole-4-carbo chloride

Other names: Dcimc chloride
4-Isoxazolecarbonyl chloride, 3-(2,6-dichlorophenyl)-5-methyl-
3-(2,6-Dichlorophenyl)-5-methylisoxazole-4-carboxylic acid chloride

Inchi: InChI=1S/C11H6Cl3NO2/c1-5-8(11(14)16)10(15-17-5)9-6(12)3-2-4-7(9)13/h2-4H,1H3

InchiKey: IZQGELJKDARDMZ-UHFFFAOYSA-N

Formula: C11H6Cl3NO2

SMILES: Cc1onc(-c2c(Cl)cccc2Cl)c1C(=O)Cl

Mol. weight [g/mol]: 290.53

Physical Properties

Property code	Value	Unit	Source
logp	4.336		Crippen Method
mcvol	176.770	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4462559&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):

Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.