

Methyl 2,5-dichlorothiophene-3-carboxylate

Inchi: InChI=1S/C6H4Cl2O2S/c1-10-6(9)3-2-4(7)11-5(3)8/h2H,1H3
InchiKey: VCXPHMKCDRPIDG-UHFFFAOYSA-N
Formula: C6H4Cl2O2S
SMILES: COC(=O)c1cc(Cl)sc1Cl
Mol. weight [g/mol]: 211.07
CAS: 145129-54-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.841		Crippen Method
mcvol	124.210	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C145129540&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/38-738-1/Methyl-2-5-dichlorothiophene-3-carboxylate.pdf>

Generated by Cheméo on 2024-05-21 12:43:24.201531538 +0000 UTC m=+18584653.122108850.

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