2-Thiophenecarboxylic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H6Cl2O2S/c12-8-4-3-7(6-9(8)13)15-11(14)10-2-1-5-16-10/h1-6H
InchiKey: BTWJLTDNAKWSDS-UHFFFAOYSA-N
Formula: C11H6Cl2O2S
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccs1
Mol. weight [g/mol]: 273.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	4.274		Crippen Method
mcvol	170.900	ml/mol	McGowan Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook

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=U308066&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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