

2-Furoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H6Cl2O3/c12-8-4-3-7(6-9(8)13)16-11(14)10-2-1-5-15-10/h1-6H
InchiKey: UJSWUBSZOMSSEA-UHFFFAOYSA-N
Formula: C11H6Cl2O3
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1ccco1
Mol. weight [g/mol]: 257.07
CAS: 116401-45-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.66		Crippen Method
logp	3.806		Crippen Method
mcvol	160.420	ml/mol	McGowan Method
rinpol	1859.00		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=C116401457&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

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