2-Furoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C11H5Cl3O3/c12-6-4-8(14)10(5-7(6)13)17-11(15)9-2-1-3-16-9/h1-5H
InchiKey: IMHATZBSQRHLIE-UHFFFAOYSA-N
Formula: C11H5Cl3O3
SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)c1ccco1
Mol. weight [g/mol]: 291.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.35		Crippen Method
logp	4.459		Crippen Method
mcvol	172.660	ml/mol	McGowan Method
rinpol	2059.00		NIST Webbook

Sources

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=U355175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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