Nicotinic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C12H7Cl2NO2/c13-10-4-3-9(6-11(10)14)17-12(16)8-2-1-5-15-7-8/h1-7H
InchiKey: GYEMZNAXCNKADB-UHFFFAOYSA-N
Formula: C12H7Cl2NO2
SMILES: O=C(Oc1ccc(Cl)c(Cl)c1)c1cccnc1
Mol. weight [g/mol]: 268.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.69		Crippen Method
logp	3.608		Crippen Method
mcvol	174.320	ml/mol	McGowan Method
rinpol	2052.00		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=U307951&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