2-Furoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C11H7ClO3/c12-8-3-5-9(6-4-8)15-11(13)10-2-1-7-14-10/h1-7H
InchiKey: ZGZHQUGYCJLSQM-UHFFFAOYSA-N
Formula: C11H7ClO3
SMILES: O=C(Oc1ccc(Cl)cc1)c1ccco1
Mol. weight [g/mol]: 222.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.98		Crippen Method
logp	3.152		Crippen Method
mcvol	148.180	ml/mol	McGowan Method
rinpol	1676.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307993&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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