

Isonicotinic acid, (4-chlorophenyl)methyl ester

Inchi: InChI=1S/C13H10ClNO2/c14-12-3-1-10(2-4-12)9-17-13(16)11-5-7-15-8-6-11/h1-8H,9H2
InchiKey: KFNLUWVOHPCBPL-UHFFFAOYSA-N
Formula: C13H10ClNO2
SMILES: O=C(OCc1ccc(Cl)cc1)c1ccncc1
Mol. weight [g/mol]: 247.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.092		Crippen Method
mcvol	176.170	ml/mol	McGowan Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		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=U308348&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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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