

Isonicotinic acid, 2-ethylcyclohexyl ester

Inchi: InChI=1S/C14H19NO2/c1-2-11-5-3-4-6-13(11)17-14(16)12-7-9-15-10-8-12/h7-11,13H,2-
InchiKey: YJQUYDHMLBSZQQ-UHFFFAOYSA-N
Formula: C14H19NO2
SMILES: CCC1CCCCC1OC(=O)c1ccncc1
Mol. weight [g/mol]: 233.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	3.207		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308362&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.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

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