

Nicotinic acid, cyclohexyl ester

Inchi: InChI=1S/C12H15NO2/c14-12(10-5-4-8-13-9-10)15-11-6-2-1-3-7-11/h4-5,8-9,11H,1-3,6-
InchiKey: DMOCRQCRHPKMRK-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: O=C(OC1CCCCC1)c1cccnc1
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	2.571		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
rinsol	1646.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U308366&Units=SI>

Legend

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

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