

Nicotinic acid, heptyl ester

Inchi: InChI=1S/C13H19NO2/c1-2-3-4-5-6-10-16-13(15)12-8-7-9-14-11-12/h7-9,11H,2-6,10H2,
InchiKey: MBYWGKLYUEAKO-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	3.209		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
rinpol	1700.00		NIST Webbook
rinpol	1700.00		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=U299858&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/120-968-4/Nicotinic-acid-heptyl-ester.pdf>

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