

Nicotinic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C18H23NO2/c20-17(16-2-1-4-19-12-16)21-5-3-18-9-13-6-14(10-18)8-15(7-13)
InchiKey: AVSOLGBUADYZAD-UHFFFAOYSA-N
Formula: C18H23NO2
SMILES: O=C(OCCC12CC3CC(CC(C3)C1)C2)c1cccnc1
Mol. weight [g/mol]: 285.38
CAS: 64140-39-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.80		Crippen Method
logp	3.845		Crippen Method
mcvol	225.560	ml/mol	McGowan Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		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=C64140392&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/97-509-0/Nicotinic-acid-2-1-adamantyl-ethyl-ester.pdf>

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