

Nicotinic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C17H21NO2/c19-16(15-2-1-3-18-10-15)20-11-17-7-12-4-13(8-17)6-14(5-12)9-
InchiKey: UUEREIOEDCBBID-UHFFFAOYSA-N
Formula: C17H21NO2
SMILES: O=C(OCC12CC3CC(CC(C3)C1)C2)c1cccnc1
Mol. weight [g/mol]: 271.35
CAS: 24813-27-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.455		Crippen Method
mcvol	211.470	ml/mol	McGowan Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C24813272&Units=SI>

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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