

Nicotinic acid, decyl ester

Inchi: InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-8-9-13-19-16(18)15-11-10-12-17-14-15/h10-12,14
InchiKey: OVSJCKDIBDNMMK-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: CCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.379		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
rinsol	1920.00		NIST Webbook
rinsol	1920.00		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=U299860&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

Latest version available from:

<https://www.chemeo.com/cid/124-897-9/Nicotinic-acid-decyl-ester.pdf>

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