Nicotinic acid, undecyl ester

Inchi: InChI=1S/C17H27NO2/c1-2-3-4-5-6-7-8-9-10-14-20-17(19)16-12-11-13-18-15-16/h11-13
InchiKey: OWEZDQWMGDOLFG-UHFFFAOYSA-N
Formula: C17H27NO2
SMILES: CCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]: 277.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	4.769		Crippen Method
mcvol	244.050	ml/mol	McGowan Method
rinpol	2121.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299975&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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