

Nicotinic acid, nonyl ester

Inchi: InChI=1S/C15H23NO2/c1-2-3-4-5-6-7-8-12-18-15(17)14-10-9-11-16-13-14/h9-11,13H,2-
InchiKey: CPDDCIYPNIRWBG-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]: 249.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.989		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299972&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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