

Isonipecotic acid, N-(octanoyl)-, ethyl ester

Inchi: InChI=1S/C16H29NO3/c1-3-5-6-7-8-9-15(18)17-12-10-14(11-13-17)16(19)20-4-2/h14H,3
InchiKey: RPXDNSYKKZHUPA-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: CCCCCCCC(=O)N1CCC(C(=O)OCC)CC1
Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	3.149		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
rinpol	2250.00		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=U361566&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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<https://www.chemeo.com/cid/21-574-1/Isonipecotic-acid-N-octanoyl-ethyl-ester.pdf>

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