

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

Inchi: InChI=1S/C17H31NO3/c1-3-5-6-7-8-9-16(19)18-12-10-15(11-13-18)17(20)21-14-4-2/h15
InchiKey: IVAHFKNSBAMNKV-UHFFFAOYSA-N
Formula: C17H31NO3
SMILES: CCCCCCCC(=O)N1CCC(C(=O)OCCC)CC1
Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.539		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpole	2357.00		NIST Webbook

Sources

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=U361567&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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