

L-Proline, N-octanoyl-, propyl ester

Inchi: InChI=1S/C16H29NO3/c1-3-5-6-7-8-11-15(18)17-12-9-10-14(17)16(19)20-13-4-2/h14H,3
InchiKey: OOTVFNNPSLCEJT-UHFFFAOYSA-N
Formula: C16H29NO3
SMILES: CCCCCC(=O)N1CCCC1C(=O)OCCC
Mol. weight [g/mol]: 283.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Crippen Method
logp	3.291		Crippen Method
mcvol	244.430	ml/mol	McGowan Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346238&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/112-954-8/L-Proline-N-octanoyl-propyl-ester.pdf>

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