

L-Proline, N-(hexanoyl)-, hexyl ester

Inchi: InChI=1S/C17H31NO3/c1-3-5-7-9-14-21-17(20)15-11-10-13-18(15)16(19)12-8-6-4-2/h15
InchiKey: VDSZTMZBBXBQAJ-UHFFFAOYSA-N
Formula: C17H31NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]: 297.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	3.681		Crippen Method
mcvol	258.520	ml/mol	McGowan Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346156&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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