

L-Proline, N-octanoyl-, ethyl ester

Inchi: InChI=1S/C15H27NO3/c1-3-5-6-7-8-11-14(17)16-12-9-10-13(16)15(18)19-4-2/h13H,3-12H
InchiKey: VTQRYTQHWQDLBF-UHFFFAOYSA-N
Formula: C15H27NO3
SMILES: CCCCCCCC(=O)N1CCCC1C(=O)OCC
Mol. weight [g/mol]: 269.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	2.901		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346237&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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