

L-Proline, N-octanoyl-, octyl ester

Inchi: InChI=1S/C21H39NO3/c1-3-5-7-9-11-13-18-25-21(24)19-15-14-17-22(19)20(23)16-12-10
InchiKey: FAQDJMAPFJJPLT-UHFFFAOYSA-N
Formula: C21H39NO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC
Mol. weight [g/mol]: 353.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.83		Crippen Method
logp	5.242		Crippen Method
mcvol	314.880	ml/mol	McGowan Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346243&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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