

L-Proline, N-octanoyl-, dodecyl ester

Inchi: InChI=1S/C25H47NO3/c1-3-5-7-9-10-11-12-13-15-17-22-29-25(28)23-19-18-21-26(23)24
InchiKey: GTJZHSSAHUXOSW-UHFFFAOYSA-N
Formula: C25H47NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCCCC
Mol. weight [g/mol]: 409.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	6.802		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
rinpol	3031.00		NIST Webbook
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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=U346247&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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/95-449-9/L-Proline-N-octanoyl-dodecyl-ester.pdf>

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