

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

Inchi: InChI=1S/C26H49NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-23-30-26(29)24-20-19-22
InchiKey: SNTZAEPOJGZEMS-UHFFFAOYSA-N
Formula: C26H49NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]: 423.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.92		Crippen Method
logp	7.192		Crippen Method
mcvol	385.330	ml/mol	McGowan Method
rinpol	3158.00		NIST Webbook
rinpol	3158.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346164&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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

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<https://www.chemeo.com/cid/86-323-8/L-Proline-N-hexanoyl-pentadecyl-ester.pdf>

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