

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

Inchi: InChI=1S/C27H51NO3/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-24-31-27(30)25-21-20
InchiKey: BVAHNWSMVAURIM-UHFFFAOYSA-N
Formula: C27H51NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]: 437.70

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.34 | | Crippen Method |
| logp | 7.582 | | Crippen Method |
| mcvol | 399.420 | ml/mol | McGowan Method |
| rinpol | 3260.00 | | NIST Webbook |
| rinpol | 3260.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U346165&Units=SI>

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/94-901-7/L-Proline-N-hexanoyl-hexadecyl-ester.pdf>

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