

L-Proline, N-octanoyl-, hexyl ester

Inchi: InChI=1S/C19H35NO3/c1-3-5-7-9-10-14-18(21)20-15-12-13-17(20)19(22)23-16-11-8-6-4
InchiKey: BTLAGCBYHPLDIK-UHFFFAOYSA-N
Formula: C19H35NO3
SMILES: CCCCCCCC(=O)N1CCCC1C(=O)OCCCCC
Mol. weight [g/mol]: 325.49

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.99 | | Crippen Method |
| logp | 4.461 | | Crippen Method |
| mcvol | 286.700 | ml/mol | McGowan Method |
| rinpol | 2425.00 | | NIST Webbook |
| rinpol | 2425.00 | | NIST Webbook |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346242&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/97-718-8/L-Proline-N-octanoyl-hexyl-ester.pdf>

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