# L-Proline, N-octanoyl-, pentyl ester

**Inchi:** InChI=1S/C18H33NO3/c1-3-5-7-8-9-13-17(20)19-14-11-12-16(19)18(21)22-15-10-6-4-2/l
**InchiKey:** ADJSDSQNNKIRDX-UHFFFAOYSA-N
**Formula:** C18H33NO3
**SMILES:** CCCCCCCC(=O)N1CCCC1C(=O)OCCCCC
**Mol. weight [g/mol]:** 311.46

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.57 | | Crippen Method |
| logp | 4.071 | | Crippen Method |
| mcvol | 272.610 | ml/mol | McGowan Method |
| rinpol | 2327.00 | | NIST Webbook |
| rinpol | 2327.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U346241&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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