

L-Proline, N-(3-cyclopentylpropionyl)-, pentyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C18H31NO3/c1-2-3-6-14-22-18(21)16-10-7-13-19(16)17(20)12-11-15-8-4-5-9- |
| InchiKey: | YKJWPZKVCQTVPU-UHFFFAOYSA-N |
| Formula: | C18H31NO3 |
| SMILES: | CCCCCOC(=O)C1CCCN1C(=O)CCC1CCCC1 |
| Mol. weight [g/mol]: | 309.44 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.22 | | Crippen Method |
| logp | 3.681 | | Crippen Method |
| mcvol | 261.750 | ml/mol | McGowan Method |
| rinpol | 2413.00 | | NIST Webbook |
| rinpol | 2413.00 | | NIST Webbook |

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=U346410&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

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|----------|-------------------------------------|
| 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/99-394-6/L-Proline-N-3-cyclopentylpropionyl-pentyl-ester.pdf>

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