

# d-Proline, n-propoxycarbonyl-, hexadecyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C25H47NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-24(27)23-19-18-2 |
| InchiKey:            | LJEKGBUAVPLPKU-UHFFFAOYSA-N  |
| Formula:             | C25H47NO4  |
| SMILES:              | CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC   |
| Mol. weight [g/mol]: | 425.64   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.57   |        | Crippen Method |
| logp          | 7.022   |        | Crippen Method |
| mcvol         | 377.110 | ml/mol | McGowan Method |
| rinpol        | 2794.00 |        | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320831&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320831&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## 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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