

# L-Proline, N-(thiophen-2-carbonyl)-, hexyl ester

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C16H23NO3S/c1-2-3-4-5-11-20-16(19)13-8-6-10-17(13)15(18)14-9-7-12-21-14 |
| InchiKey:            | IDMSVDZKNLBESY-UHFFFAOYSA-N                                                      |
| Formula:             | C16H23NO3S                                                                       |
| SMILES:              | CCCCCOC(=O)C1CCCN1C(=O)c1cccs1                                                   |
| Mol. weight [g/mol]: | 309.42                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.01   |        | Crippen Method |
| logp          | 3.476   |        | Crippen Method |
| mcvol         | 241.320 | ml/mol | McGowan Method |
| rinpol        | 2501.00 |        | NIST Webbook   |
| rinpol        | 2501.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| 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=U346372&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U346372&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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<https://www.chemeo.com/cid/122-602-7/L-Proline-N-thiophen-2-carbonyl-hexyl-ester.pdf>

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