

L-Proline, N-(thiophen-2-carbonyl)-, heptyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C17H25NO3S/c1-2-3-4-5-6-12-21-17(20)14-9-7-11-18(14)16(19)15-10-8-13-22 |
| InchiKey: | HPKNBQBOKWQGHJ-UHFFFAOYSA-N |
| Formula: | C17H25NO3S |
| SMILES: | CCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1 |
| Mol. weight [g/mol]: | 323.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.43 | | Crippen Method |
| logp | 3.866 | | Crippen Method |
| mcvol | 255.410 | ml/mol | McGowan Method |
| rinpol | 2602.00 | | NIST Webbook |
| rinpol | 2602.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.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=U346373&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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