

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

Inchi: InChI=1S/C14H19NO3S/c1-2-3-9-18-14(17)11-6-4-8-15(11)13(16)12-7-5-10-19-12/h5,7,
InchiKey: UEEQAVNRYZDWPC-UHFFFAOYSA-N
Formula: C14H19NO3S
SMILES: CCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 281.37

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.17 | | Crippen Method |
| logp | 2.696 | | Crippen Method |
| mcvol | 213.140 | ml/mol | McGowan Method |
| rinpol | 2301.00 | | NIST Webbook |
| rinpol | 2301.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346370&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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