

2-Thiophenecarboxamide, N-(hept-2-yl)-

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|-----------------------------|--|
| Inchi: | InChI=1S/C12H19NOS/c1-3-4-5-7-10(2)13-12(14)11-8-6-9-15-11/h6,8-10H,3-5,7H2,1-2H |
| InchiKey: | FCLHURNQXYAFJF-UHFFFAOYSA-N |
| Formula: | C12H19NOS |
| SMILES: | CCCCC(C)NC(=O)c1cccs1 |
| Mol. weight [g/mol]: | 225.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.20 | | Crippen Method |
| logp | 3.447 | | Crippen Method |
| mcvol | 188.380 | ml/mol | McGowan Method |
| rinpola | 1857.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407026&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| rinpola: | Non-polar retention indices |

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