

Furan-2-carboxamide, N-butyl-N-heptyl-

Inchi: InChI=1S/C16H27NO2/c1-3-5-7-8-9-13-17(12-6-4-2)16(18)15-11-10-14-19-15/h10-11,14
InchiKey: KXXUXKHAVAPJXKK-UHFFFAOYSA-N
Formula: C16H27NO2
SMILES: CCCCCCN(CCCC)C(=O)c1ccco1
Mol. weight [g/mol]: 265.39

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -9.12 | | Crippen Method |
| logp | 4.492 | | Crippen Method |
| mcvol | 234.260 | ml/mol | McGowan Method |
| rinpol | 2522.00 | | NIST Webbook |
| rinpol | 2522.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415647&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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