

2-Furancarboxamide, N-pentyl-

Inchi: InChI=1S/C10H15NO2/c1-2-3-4-7-11-10(12)9-6-5-8-13-9/h5-6,8H,2-4,7H2,1H3,(H,11,12)
InchiKey: WOFOKONYZCFKNF-UHFFFAOYSA-N
Formula: C10H15NO2
SMILES: CCCCCNC(=O)c1ccco1
Mol. weight [g/mol]: 181.23

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.22 | | Crippen Method |
| logp | 2.200 | | Crippen Method |
| mcvol | 149.720 | ml/mol | McGowan Method |
| rinpol | 1562.00 | | NIST Webbook |
| rinpol | 1562.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.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=U407243&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/90-947-1/2-Furancarboxamide-N-pentyl.pdf>

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