

2-Furancarboxamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C11H8FNO2/c12-8-3-5-9(6-4-8)13-11(14)10-2-1-7-15-10/h1-7H,(H,13,14)
InchiKey: AQQZKDFBNBVLHX-UHFFFAOYSA-N
Formula: C11H8FNO2
SMILES: O=C(Nc1ccc(F)cc1)c1ccco1
Mol. weight [g/mol]: 205.19

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.51 | | Crippen Method |
| logp | 2.671 | | Crippen Method |
| mcvol | 141.820 | ml/mol | McGowan Method |
| rinpole | 1699.00 | | NIST Webbook |
| rinpole | 1699.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307035&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
rinpole: Non-polar retention indices

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