

2-Furoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C11H3F5O3/c12-5-6(13)8(15)10(9(16)7(5)14)19-11(17)4-2-1-3-18-4/h1-3H
InchiKey: UIHCMTCYMQANRT-UHFFFAOYSA-N
Formula: C11H3F5O3
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1ccco1
Mol. weight [g/mol]: 278.13

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.95 | | Crippen Method |
| logp | 3.194 | | Crippen Method |
| mcvol | 144.790 | ml/mol | McGowan Method |
| rinsol | 1385.00 | | 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=U355170&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
rinsol: Non-polar retention indices

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