

2-Furoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

| | |
|----------------------|---|
| Inchi: | InChI=1S/C10H6F8O3/c11-7(12)9(15,16)10(17,18)8(13,14)4-21-6(19)5-2-1-3-20-5/h1-3, |
| InchiKey: | IKKGIAHJHOPGRE-UHFFFAOYSA-N |
| Formula: | C10H6F8O3 |
| SMILES: | O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccco1 |
| Mol. weight [g/mol]: | 326.14 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.38 | | Crippen Method |
| logp | 3.607 | | Crippen Method |
| mcvol | 159.770 | ml/mol | McGowan Method |
| rinsol | 1211.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355167&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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