

L-Proline, N-(pentafluorobenzoyl)-, propyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H14F5NO3/c1-2-6-24-15(23)7-4-3-5-21(7)14(22)8-9(16)11(18)13(20)12(19) |
| InchiKey: | FFNZJZLABNDQQQ-UHFFFAOYSA-N |
| Formula: | C15H14F5NO3 |
| SMILES: | CCCOC(=O)C1CCCN1C(=O)c1c(F)c(F)c(F)c(F)c1F |
| Mol. weight [g/mol]: | 351.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.65 | | Crippen Method |
| logp | 2.940 | | Crippen Method |
| mcvol | 215.430 | ml/mol | McGowan Method |
| rinpol | 1908.00 | | NIST Webbook |
| rinpol | 1908.00 | | 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=U346291&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 |

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<https://www.chemeo.com/cid/117-625-8/L-Proline-N-pentafluorobenzoyl-propyl-ester.pdf>

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