

Isonipecotic acid, N-(4-fluorobenzoyl)-, butyl ester

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|----------------------|--|
| Inchi: | InChI=1S/C17H22FNO3/c1-2-3-12-22-17(21)14-8-10-19(11-9-14)16(20)13-4-6-15(18)7-5 |
| InchiKey: | UEWSLCIHCLUWND-UHFFFAOYSA-N |
| Formula: | C17H22FNO3 |
| SMILES: | CCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1 |
| Mol. weight [g/mol]: | 307.36 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.81 | | Crippen Method |
| logp | 3.021 | | Crippen Method |
| mcvol | 236.530 | ml/mol | McGowan Method |
| rinpola | 2420.00 | | NIST Webbook |

Sources

| | |
|-----------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U361070&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| rinpola: | Non-polar retention indices |

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