

Isonipectic acid, N-(2,4-difluorobenzoyl)-, heptyl ester

Inchi: InChI=1S/C20H27F2NO3/c1-2-3-4-5-6-13-26-20(25)15-9-11-23(12-10-15)19(24)17-8-7-1
InchiKey: IJLCCPDTMDRPBY-UHFFFAOYSA-N
Formula: C20H27F2NO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2F)CC1
Mol. weight [g/mol]: 367.43

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.40 | | Crippen Method |
| logp | 4.331 | | Crippen Method |
| mcvol | 280.570 | ml/mol | McGowan Method |
| rinsol | 2661.00 | | NIST Webbook |
| rinsol | 2661.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U361370&Units=SI>

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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