

Isonipecotinoylisonipecotic acid, N'-pentafluorobenzoyl-, isoheptyl ester

Inchi: InChI=1S/C25H31F5N2O4/c1-14(2)4-3-13-36-25(35)16-7-11-31(12-8-16)23(33)15-5-9-3
InchiKey: JVCLCYKMHGBCID-UHFFFAOYSA-N
Formula: C25H31F5N2O4
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3c(F)c(F)c(F)c(F)c3F)CC2)CC1
Mol. weight [g/mol]: 518.52

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.24 | | Crippen Method |
| logp | 4.452 | | Crippen Method |
| mcvol | 357.020 | ml/mol | McGowan Method |
| rinpola | 3544.00 | | 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=U361238&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
rinpola: Non-polar retention indices

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