

Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, isohexyl ester

InChI: InChI=1S/C20H25F4NO3/c1-13(2)4-3-11-28-19(27)14-7-9-25(10-8-14)18(26)16-12-15(2)
InChIKey: ROUGZQVIFROUNB-UHFFFAOYSA-N
Formula: C20H25F4NO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 403.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.51 | | Crippen Method |
| logp | 4.676 | | Crippen Method |
| mcvol | 284.110 | ml/mol | McGowan Method |
| rinpola | 2452.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361332&Units=SI>
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>

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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