

Isonipecotic acid, N-(3-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C26H38F3NO3/c1-2-3-4-5-6-7-8-9-10-11-19-33-25(32)21-15-17-30(18-16-21)2
InchiKey: FSKLHMAJKXEPFK-UHFFFAOYSA-N
Formula: C26H38F3NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 469.58

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.93 | | Crippen Method |
| logp | 7.022 | | Crippen Method |
| mcvol | 366.880 | ml/mol | McGowan Method |
| rinpol | 3159.00 | | NIST Webbook |
| rinpol | 3159.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361550&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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