

Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, decyl ester

Inchi: InChI=1S/C25H33F6NO3/c1-2-3-4-5-6-7-8-9-16-35-23(34)18-12-14-32(15-13-18)22(33)2
InchiKey: OPMHEUNIEKWXQX-UHFFFAOYSA-N
Formula: C25H33F6NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 509.52

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.20 | | Crippen Method |
| logp | 7.260 | | Crippen Method |
| mcvol | 358.100 | ml/mol | McGowan Method |
| rinpol | 2753.00 | | NIST Webbook |
| rinpol | 2753.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361210&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
rinpol: Non-polar retention indices

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