

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

Inchi: InChI=1S/C27H40F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-20-34-26(33)22-16-18-31(19-17-20)
InchiKey: KSQJOPVIKKDLBO-UHFFFAOYSA-N
Formula: C27H40F3NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 483.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	7.412		Crippen Method
mcvol	380.970	ml/mol	McGowan Method
rinpole	3261.00		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=U361551&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/11-675-0/Isonipecotic-acid-N-3-trifluoromethylbenzoyl-tridecyl-ester.pdf>

Generated by Cheméo on 2024-04-19 14:49:35.061343813 +0000 UTC m=+15827423.981921124.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.