

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

Inchi: InChI=1S/C28H42F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-35-27(34)23-17-19-32(20-1
InchiKey: KLENRVRIPPMERB-UHFFFAOYSA-N
Formula: C28H42F3NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 497.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.77		Crippen Method
logp	7.802		Crippen Method
mcvol	395.060	ml/mol	McGowan Method
rinpol	3361.00		NIST Webbook
rinpol	3361.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361552&Units=SI>

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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