

Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: [InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-36-27\(35\)22-14-16-33\(17-18\)19-20-21](https://www.ebi.ac.uk/chembl/compound/15/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-36-27(35)22-14-16-33(17-18)19-20-21)
InChIKey: AQEKPCXXZVKMRJ-UHFFFAOYSA-N

Formula: C28H41F4NO3

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 515.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.10		Crippen Method
logp	7.941		Crippen Method
mcvol	396.830	ml/mol	McGowan Method
rinpole	3246.00		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=U361458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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