

Isonipectic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1
InChIKey: HNFFYYBIGGUTKC-UHFFFAOYSA-N

Formula: C₂₈H₄₁F₄NO₃

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(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
rinpol	3350.00		NIST Webbook
rinpol	3350.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361478&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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