

Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-36-27(35)22-17-19-33(20-18-22)26(34)23-15-14-16-24(25(23)29)28(30,31)32/h14-16,22H,2-13,17-21H2,1H3

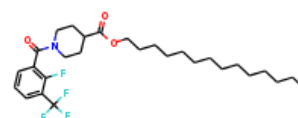
InChI Key: KCXVRHFMRGOJBU-UHFFFAOYSA-N

Formula: C28H41F4NO3

SMILES:

CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)CC1

Molecular Weight: 515.62



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	7.94		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-36-27\(35\)22-17-19-33\(20-18-22\)26\(34\)23-15-14-16-24\(25\(23\)29\)28\(30,31\)32/h14-16,22H,2-13,17-21H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-36-27(35)22-17-19-33(20-18-22)26(34)23-15-14-16-24(25(23)29)28(30,31)32/h14-16,22H,2-13,17-21H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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