

Isonipectic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, tridecyl ester

InChI: InChI=1S/C27H39F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-35-26(34)21-15-17-32(18-16-21)25(33)23-20-22(27(29,30)31)13-14-24(23)28/h13-14,20-21H,2-12,15-19H2,1H3

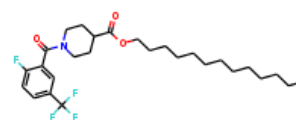
InChI Key: ALPUJNYKFBAMBA-UHFFFAOYSA-N

Formula: C27H39F4NO3

SMILES:

CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1

Molecular Weight: 501.60



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	7.55		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H39F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-35-26\(34\)21-15-17-32\(18-16-21\)25\(33\)23-20-22\(27\(29,30\)31\)13-14-24\(23\)28/h13-14,20-21H,2-12,15-19H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H39F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-35-26(34)21-15-17-32(18-16-21)25(33)23-20-22(27(29,30)31)13-14-24(23)28/h13-14,20-21H,2-12,15-19H2,1H3)

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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