

Isonipectic acid, N-(3-trifluoromethylbenzoyl)-, pentadecyl

Inchi:
ester

InChI=1S/C29H44F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-22-36-28(35)24-18-20-33(2

InchiKey:

INVCKMRXPAHYMC-UHFFFAOYSA-N

Formula:

C29H44F3NO3

SMILES:

CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]:

511.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.19		Crippen Method
logp	8.192		Crippen Method
mcvol	409.150	ml/mol	McGowan Method
rinpole	3479.00		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=U361553&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

Latest version available from:

<https://www.chemeo.com/cid/59-803-5/Isonipectic-acid-N-3-trifluoromethylbenzoyl-pentadecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 07:03:22.132665734 +0000 UTC m=+16145051.053243052.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.