

Isonipectic acid, N-(3-trifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C25H36F3NO3/c1-2-3-4-5-6-7-8-9-10-18-32-24(31)20-14-16-29(17-15-20)23(3)
InchiKey: KGWWJTYARVRJGI-UHFFFAOYSA-N
Formula: C25H36F3NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 455.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	6.632		Crippen Method
mcvol	352.790	ml/mol	McGowan Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		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=U361549&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
rinpol: Non-polar retention indices

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