

Isonipecotic acid, N-(2-fluoro-6-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)CC1
InChIKey: UXRDLHDGGLMHNE-UHFFFAOYSA-N

Formula: C₂₈H₄₁F₄NO₃

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)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
rinpole	3368.00		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=U361296&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/13-334-6/Isonipecotic-acid-N-2-fluoro-6-trifluoromethylbenzoyl-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-23 07:53:49.880116306 +0000 UTC m=+16148078.800693618.

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