Isonipecotic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C26H37F4NO3/c1-2-3-4-5-6-7-8-9-10-11-18-34-25(33)20-14-16-31(17-15-20)2
InchiKey: WJCMBEXYZCCRJI-UHFFFAOYSA-N
Formula: C26H37F4NO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1
Mol. weight [g/mol]: 487.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	7.161		Crippen Method
mcvol	368.650	ml/mol	McGowan Method
rinpol	3149.00		NIST Webbook
rinpol	3149.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U361476&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/68-957-5/Isonipecotic-acid-N-3-fluoro-4-trifluoromethylbenzoyl-dodecyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:54:31.782981335 +0000 UTC m=+3304134.419950584.

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