

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

InChI: InChI=1S/C26H37F4NO3/c1-2-3-4-5-6-7-8-9-10-11-19-34-25(33)20-15-17-31(18-16-20)2
InChIKey: NYECCTGLJFSCAJ-UHFFFAOYSA-N

Formula: C26H37F4NO3

SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)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	3163.00		NIST Webbook
rinpol	3163.00		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=U361295&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/121-686-6/Isonipecotic-acid-N-2-fluoro-6-trifluoromethylbenzoyl-dodecyl-ester.pdf>

Generated by Cheméo on 2026-03-07 17:43:31.273191561 +0000 UTC m=+3303102.966260797.

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