

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

InChI: InChI=1S/C23H31F4NO3/c1-2-3-4-5-6-7-8-16-31-22(30)17-12-14-28(15-13-17)21(29)20
InChIKey: TYBWJBOQCDKRSU-UHFFFAOYSA-N

Formula: C₂₃H₃₁F₄NO₃

SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)CC1

Mol. weight [g/mol]: 445.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	5.991		Crippen Method
mcvol	326.380	ml/mol	McGowan Method
rinpol	2837.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361292&Units=SI>

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

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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.cheméo.com/cid/38-477-1/Isonipecotic-acid-N-2-fluoro-6-trifluoromethylbenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2025-12-05 23:22:54.142231582 +0000 UTC m=+4725171.672272237.

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