

Isonipectic acid, N-(2-fluoro-3-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)18
InChIKey: NBULHZGKGXRSR-UHFFFAOYSA-N
Formula: C23H31F4NO3
SMILES: CCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)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
rinpole	2832.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361315&Units=SI>

Legend

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

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