

Isonipectic acid, N-(2-fluoro-6-trifluoromethylbenzoyl)- undecyl ester

InChI: InChI=1S/C25H35F4NO3/c1-2-3-4-5-6-7-8-9-10-18-33-24(32)19-14-16-30(17-15-19)23(31)1-2
InChIKey: CTRCUJDNJBMEPP-UHFFFAOYSA-N

Formula: C₂₅H₃₅F₄NO₃
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)CC1
Mol. weight [g/mol]: 473.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.85		Crippen Method
logp	6.771		Crippen Method
mcvol	354.560	ml/mol	McGowan Method
rinpole	3060.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361294&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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