

Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: [InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-36-27\(35\)22-16-18-33\(19-14-15\)/q>>1](#)
InChIKey: [LNQNFYCCGJMMF-UHFFFAOYSA-N](#)

Formula: C₂₈H₄₁F₄NO₃
SMILES: [CCCCCCCCCCCCCOC\(=O\)C1CCN\(C\(=O\)c2cc\(F\)ccc2C\(F\)\(F\)F\)CC1](#)
Mol. weight [g/mol]: 515.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.10		Crippen Method
logp	7.941		Crippen Method
mcvol	396.830	ml/mol	McGowan Method
rinpole	3315.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361341&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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