

Isonipecotic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, propyl ester

InChI: InChI=1S/C17H19F4NO3/c1-2-9-25-16(24)11-5-7-22(8-6-11)15(23)13-10-12(17(19,20)21)3
InChIKey: VPMSJEGKCIVQTA-UHFFFAOYSA-N
Formula: C17H19F4NO3
SMILES: CCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1
Mol. weight [g/mol]: 361.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	3.650		Crippen Method
mcvol	241.840	ml/mol	McGowan Method
rinpole	2182.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361386&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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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