Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C21H28F3NO3/c1-2-3-4-5-8-15-28-20(27)16-11-13-25(14-12-16)19(26)17-9-6-

InchiKey: APGMWSDFUGVVPS-UHFFFAOYSA-N

Formula: C21H28F3NO3

SMILES: CCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1

Mol. weight [g/mol]: 399.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	5.071		Crippen Method
mcvol	296.430	ml/mol	McGowan Method
rinpol	2679.00		NIST Webbook
rinpol	2679.00		NIST Webbook

Sources

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

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=U361492&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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