

Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, hexyl ester

InChI: InChI=1S/C20H25F4NO3/c1-2-3-4-5-12-28-19(27)14-8-10-25(11-9-14)18(26)16-7-6-15(2)
InChIKey: FHWHSNORFCAJPX-UHFFFAOYSA-N

Formula: C20H25F4NO3

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1

Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	4.820		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361246&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
rinpol:	Non-polar retention indices

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