

Isonipecotic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, propyl

Inchi:
ester

InChI=1S/C17H19F4NO3/c1-2-9-25-16(24)11-5-7-22(8-6-11)15(23)13-4-3-12(18)10-14(1

InchiKey: SJJAHMFBMBCBWRN-UHFFFAOYSA-N

Formula: C17H19F4NO3

SMILES: CCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)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	2186.00		NIST Webbook
rinpole	2186.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361241&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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