

Isonipecotinoylisonipecotic acid, N'-(2,5-di(trifluoromethyl)benzoyl)-, ethyl ester

Inchi: InChI=1S/C23H26F6N2O4/c1-2-35-21(34)15-7-11-30(12-8-15)19(32)14-5-9-31(10-6-14)
InchiKey: IHNGGRDMCIUNRX-UHFFFAOYSA-N
Formula: C23H26F6N2O4
SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(C(F)(F)F)ccc3C(F)(F)F)CC2)CC1
Mol. weight [g/mol]: 508.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	4.378		Crippen Method
mcvol	330.610	ml/mol	McGowan Method
rinpol	3082.00		NIST Webbook
rinpol	3082.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361218&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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