

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

Other names:	Isonipecotinoylisonipecotic acid, N'-(2,5-di(trifluoromethyl)benzoyl)-, ester
Inchi:	InChI=1S/C24H28F6N2O4/c1-2-13-36-22(35)16-7-11-31(12-8-16)20(33)15-5-9-32(10-6-
InchiKey:	DZSFPOIUUVVHR-UHFFFAOYSA-N
Formula:	C24H28F6N2O4
SMILES:	CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(C(F)(F)F)ccc3C(F)(F)F)CC2)CC1
Mol. weight [g/mol]:	522.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	4.768		Crippen Method
mcvol	344.700	ml/mol	McGowan Method
rinsol	3186.00		NIST Webbook

Sources

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=U361219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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