

Isonipecotic acid, N-pentafluorobenzoyl-, dodecyl ester

Inchi:	InChI=1S/C25H34F5NO3/c1-2-3-4-5-6-7-8-9-10-11-16-34-25(33)17-12-14-31(15-13-17)2
InchiKey:	UFKRSWGNAYDFGC-UHFFFAOYSA-N
Formula:	C25H34F5NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]:	491.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	6.698		Crippen Method
mcvol	356.330	ml/mol	McGowan Method
rinpola	3018.00		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=U361232&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
rinpola:	Non-polar retention indices

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