

Isonipecotic acid, N-(4-fluorobenzoyl)-, tridecyl ester

Inchi:	InChI=1S/C26H40FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-21-31-26(30)23-17-19-28(20-18-23
InchiKey:	HGNMJFASGCOOFH-UHFFFAOYSA-N
Formula:	C26H40FNO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	433.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.58		Crippen Method
logp	6.532		Crippen Method
mcvol	363.340	ml/mol	McGowan Method
rinpole	3372.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpole:	Non-polar retention indices

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