

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

Inchi:	InChI=1S/C16H20FNO3/c1-2-11-21-16(20)13-7-9-18(10-8-13)15(19)12-3-5-14(17)6-4-12
InchiKey:	CYUPQDFRQMYIQS-UHFFFAOYSA-N
Formula:	C16H20FNO3
SMILES:	CCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	293.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.631		Crippen Method
mcvol	222.440	ml/mol	McGowan Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U361068&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/30-904-4/Isonipecotic-acid-N-4-fluorobenzoyl-propyl-ester.pdf>

Generated by Cheméo on 2025-12-05 12:50:39.22799205 +0000 UTC m=+4687236.758032705.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.