

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

Inchi:	InChI=1S/C20H28FNO3/c1-2-3-4-5-6-15-25-20(24)17-11-13-22(14-12-17)19(23)16-7-9-1
InchiKey:	DVTOQNAZQCIUOM-UHFFFAOYSA-N
Formula:	C20H28FNO3
SMILES:	CCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2)CC1
Mol. weight [g/mol]:	349.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	4.191		Crippen Method
mcvol	278.800	ml/mol	McGowan Method
rinpola	2728.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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