Isonicotinic acid, 3-pentadecyl ester

Inchi:	InChI=1S/C21H35NO2/c1-3-5-6-7-8-9-10-11-12-13-14-20(4-2)24-21(23)19-15-17-22-18-
InchiKey:	QHRRTMQWGZVHPP-UHFFFAOYSA-N
Formula:	C21H35NO2
SMILES:	CCCCCCCCCCCCC(CC)OC(=O)c1ccncc1
Mol. weight [g/mol]:	333.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	6.328		Crippen Method
mcvol	300.410	ml/mol	McGowan Method

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=U299902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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