

Isonicotinic acid, decyl ester

Inchi:	InChI=1S/C16H25NO2/c1-2-3-4-5-6-7-8-9-14-19-16(18)15-10-12-17-13-11-15/h10-13H,2
InchiKey:	FCQDHSSRNVWVOE-UHFFFAOYSA-N
Formula:	C16H25NO2
SMILES:	CCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]:	263.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.379		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
rinpola	1908.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U299885&Units=SI

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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<https://www.chemeo.com/cid/21-253-7/Isonicotinic-acid-decyl-ester.pdf>

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