Isonicotinic acid, dodec-9-ynyl ester

Inchi:	InChI=1S/C18H25NO2/c1-2-3-4-5-6-7-8-9-10-11-16-21-18(20)17-12-14-19-15-13-17/h12
InchiKey:	NPMYSCXGBSPJKR-UHFFFAOYSA-N
Formula:	C18H25NO2
SMILES:	CCC#CCCCCCCCCOC(=O)c1ccncc1
Mol. weight [g/mol]:	287.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.383		Crippen Method
mcvol	249.540	ml/mol	McGowan Method
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U299968&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

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