

Pentadecan-1-ol, nicotinate

Other names:	Nicotinic acid, pentadecyl ester
Inchi:	InChI=1S/C21H35NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-24-21(23)20-16-15-17-22-
InchiKey:	DDAXSEWWNPAMQN-UHFFFAOYSA-N
Formula:	C21H35NO2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	333.51
CAS:	124424-97-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	6.330		Crippen Method
mcvol	300.410	ml/mol	McGowan Method
rinsol	2538.00		NIST Webbook
rinsol	2538.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124424971&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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