

Tetradecan-1-ol, nicotinate

Other names:	Nicotinic acid, tetradecyl ester
Inchi:	InChI=1S/C20H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-23-20(22)19-15-14-16-21-18-
InchiKey:	TVGLGJWCZSCAEM-UHFFFAOYSA-N
Formula:	C20H33NO2
SMILES:	CCCCCCCCCCCCCOOC(=O)c1cccnc1
Mol. weight [g/mol]:	319.48
CAS:	273203-62-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.92		Crippen Method
logp	5.939		Crippen Method
mcvol	286.320	ml/mol	McGowan Method
rinpola	2434.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C273203626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpola:	Non-polar retention indices

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