

Isonicotinic acid, 5-tetradecyl ester

Inchi:	InChI=1S/C20H33NO2/c1-3-5-7-8-9-10-11-13-19(12-6-4-2)23-20(22)18-14-16-21-17-15-
InchiKey:	SEQZNIZWQLNDOZ-UHFFFAOYSA-N
Formula:	C20H33NO2
SMILES:	CCCCCCCCC(CCCC)OC(=O)c1ccncc1
Mol. weight [g/mol]:	319.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.938		Crippen Method
mcvol	286.320	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299900&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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