

Isonicotinic acid, 2-tetradecyl ester

Inchi:	InChI=1S/C20H33NO2/c1-3-4-5-6-7-8-9-10-11-12-13-18(2)23-20(22)19-14-16-21-17-15-
InchiKey:	XZMXTTIGWHVCNR-UHFFFAOYSA-N
Formula:	C20H33NO2
SMILES:	CCCCCCCCCCCC(C)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

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=U299897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-518-1/Isonicotinic-acid-2-tetradecyl-ester.pdf>

Generated by Cheméo on 2024-04-27 06:29:02.716904724 +0000 UTC m=+16488591.637482036.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.