

Octadecyl nicotinate

Other names:	Nicotinic acid, octadecyl ester
Inchi:	InChI=1S/C24H41NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-27-24(26)23-19-
InchiKey:	LCMBGJRROPDVAA-UHFFFAOYSA-N
Formula:	C24H41NO2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)c1cccnc1
Mol. weight [g/mol]:	375.59
CAS:	33233-29-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	7.500		Crippen Method
mcvol	342.680	ml/mol	McGowan Method
rinpol	2846.00		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=C33233293&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

Latest version available from:

<https://www.chemeo.com/cid/64-024-4/Octadecyl-nicotinate.pdf>

Generated by Cheméo on 2025-12-05 23:54:27.601694677 +0000 UTC m=+4727065.131735343.

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