

2,6-Pyridinedicarboxylic acid, nonyl tridecyl ester

Inchi:	InChI=1S/C29H49NO4/c1-3-5-7-9-11-12-13-14-16-18-20-25-34-29(32)27-23-21-22-26(30)
InchiKey:	GXECIOZFAATLQH-UHFFFAOYSA-N
Formula:	C29H49NO4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCC)n1
Mol. weight [g/mol]:	475.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.09		Crippen Method
logp	8.457		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3269.00		NIST Webbook
rinpol	3269.00		NIST Webbook

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=U368827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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