

2,6-Pyridinedicarboxylic acid, dodecyl tridecyl ester

Inchi:	InChI=1S/C32H55NO4/c1-3-5-7-9-11-13-15-17-19-21-23-28-37-32(35)30-26-24-25-29(3
InchiKey:	JWIRYKBIGXOXTI-UHFFFAOYSA-N
Formula:	C32H55NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCC)n1
Mol. weight [g/mol]:	517.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.35		Crippen Method
logp	9.627		Crippen Method
mcvol	462.840	ml/mol	McGowan Method
rinsol	3534.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinsol:	Non-polar retention indices

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