

2,6-Pyridinedicarboxylic acid, dodecyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C30H51NO5/c1-4-6-8-10-11-12-13-14-15-17-25-35-29(32)27-22-18-23-28(31-2
InchiKey: ZYRSSEQSBCTWEN-UHFFFAOYSA-N
Formula: C30H51NO5
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OC(CCCCC)CCCOC)n1
Mol. weight [g/mol]: 505.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.71		Crippen Method
logp	8.082		Crippen Method
mcvol	440.530	ml/mol	McGowan Method
rinpola	3269.00		NIST Webbook
rinpola	3269.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U369252&Units=SI>

Legend

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

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