

2,6-Pyridinedicarboxylic acid, decyl tetradecyl ester

Inchi: InChI=1S/C31H53NO4/c1-3-5-7-9-11-13-14-15-16-18-20-22-27-36-31(34)29-25-23-24-28
InchiKey: AYOMNVDUCBVHOD-UHFFFAOYSA-N
Formula: C31H53NO4
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCC)n1
Mol. weight [g/mol]: 503.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.93		Crippen Method
logp	9.237		Crippen Method
mcvol	448.750	ml/mol	McGowan Method
rinpola	3433.00		NIST Webbook
rinpola	3433.00		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=U368816&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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