2,6-Pyridinedicarboxylic acid, didodecyl ester

Inchi: InChI=1S/C31H53NO4/c1-3-5-7-9-11-13-15-17-19-21-26-35-30(33)28-24-23-25-29(32-28
InchiKey: DCTIQGQGKWAWCT-UHFFFAOYSA-N
Formula: C31H53NO4
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCC)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
rinpol	3448.00		NIST Webbook
rinpol	3448.00		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=U368994&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

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