

2,6-Pyridinedicarboxylic acid, dodecyl undecyl ester

Inchi: InChI=1S/C30H51NO4/c1-3-5-7-9-11-13-15-17-19-21-26-35-30(33)28-24-22-23-27(31-29)4-6-2
InchiKey: APUIQLLBJHRZHV-UHFFFAOYSA-N
Formula: C30H51NO4
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCC)n1
Mol. weight [g/mol]: 489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.51		Crippen Method
logp	8.847		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpol	3337.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368993&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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