

2,6-Pyridinedicarboxylic acid, 2-octylpentadecyl ester

Inchi: InChI=1S/C30H51NO4/c1-4-6-8-10-11-12-13-14-15-16-17-18-20-25-34-29(32)27-23-21-2
InchiKey: FNPIRUJGYMUNQ-UHFFFAOYSA-N
Formula: C30H51NO4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCCC)n1
Mol. weight [g/mol]: 489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	8.845		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpol	3255.00		NIST Webbook
rinpol	3255.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368311&Units=SI>
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>

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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