2,6-Pyridinedicarboxylic acid, pentadecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C30H51NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-22-34-28(32)26-20-19-21
InchiKey: FZISFGUBPBKSSB-UHFFFAOYSA-N
Formula: C30H51NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1
Mol. weight [g/mol]: 489.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.03		Crippen Method
logp	8.559		Crippen Method
mcvol	434.660	ml/mol	McGowan Method
rinpol	3231.00		NIST Webbook
rinpol	3231.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U368801&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

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