2,6-Pyridinedicarboxylic acid, neopentyl tetradecyl ester

Inchi: InChI=1S/C26H43NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-20-30-24(28)22-18-17-19-23(

InchiKey: VVCTYDYPZMLCCQ-UHFFFAOYSA-N

Formula: C26H43NO4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1

Mol. weight [g/mol]: 433.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	7.142		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
rinpol	2998.00		NIST Webbook
rinpol	2998.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369010&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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