

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

Inchi: InChI=1S/C33H57NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-37-31(35)29
InchiKey: IMBYBPRCOFNTFH-UHFFFAOYSA-N
Formula: C33H57NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1
Mol. weight [g/mol]: 531.81

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.29		Crippen Method
logp	9.729		Crippen Method
mcvol	476.930	ml/mol	McGowan Method
rinpole	3498.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368804&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
rinpole: Non-polar retention indices

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