

2,6-Pyridinedicarboxylic acid, hexyl pentadecyl ester

Inchi: InChI=1S/C28H47NO4/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-24-33-28(31)26-22-20-2
InchiKey: VLDSVQVUENOWGP-UHFFFAOYSA-N
Formula: C28H47NO4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1
Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.68		Crippen Method
logp	8.067		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinpola	3216.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368783&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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