

2,6-Pyridinedicarboxylic acid, dodecyl 2-octyl ester

Inchi: InChI=1S/C27H45NO4/c1-4-6-8-10-11-12-13-14-15-17-22-31-26(29)24-20-18-21-25(28-2)
InchiKey: YMDIBSLJXZFLBN-UHFFFAOYSA-N
Formula: C27H45NO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCC)n1
Mol. weight [g/mol]: 447.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.37		Crippen Method
logp	7.675		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
rinpole	3065.00		NIST Webbook
rinpole	3065.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368308&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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