

2,6-Pyridinedicarboxylic acid, pentadecyl 2-pentyl ester

Inchi:	InChI=1S/C27H45NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-22-31-26(29)24-20-18-21
InchiKey:	OVGFDVQXPSIASH-UHFFFAOYSA-N
Formula:	C27H45NO4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCC)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	3101.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368345&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/50-831-3/2-6-Pyridinedicarboxylic-acid-pentadecyl-2-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-27 22:15:24.440416333 +0000 UTC m=+16545373.360993646.

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