

2,6-Pyridinedicarboxylic acid, decyl undecyl ester

Inchi:	InChI=1S/C28H47NO4/c1-3-5-7-9-11-13-15-17-19-24-33-28(31)26-22-20-21-25(29-26)27
InchiKey:	MPIUHRVCSGLWGM-UHFFFAOYSA-N
Formula:	C28H47NO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCCCC)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	3205.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368813&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
mcvola:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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