

2,6-Pyridinedicarboxylic acid, 3-methylbutyl pentadecyl ester

Inchi:	InChI=1S/C27H45NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-31-26(29)24-18-17-19-2
InchiKey:	MWBIQJWPTPTBTP-UHFFFAOYSA-N
Formula:	C27H45NO4
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)C)n1
Mol. weight [g/mol]:	447.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.02		Crippen Method
logp	7.533		Crippen Method
mcvol	392.390	ml/mol	McGowan Method
rinpola	3134.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368327&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
rinpola:	Non-polar retention indices

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