

2,6-Pyridinedicarboxylic acid, heptadecyl neopentyl ester

Inchi:	InChI=1S/C29H49NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-33-27(31)25-21
InchiKey:	VVNGVGKCASZOQM-UHFFFAOYSA-N
Formula:	C29H49NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
Mol. weight [g/mol]:	475.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.85		Crippen Method
logp	8.313		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpola	3207.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369013&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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