

# 2,6-Pyridinedicarboxylic acid, dineopentyl ester

Inchi:	InChI=1S/C17H25NO4/c1-16(2,3)10-21-14(19)12-8-7-9-13(18-12)15(20)22-11-17(4,5)6/1
InchiKey:	RFOVDJMEDCUHLV-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	CC(C)(C)COC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
Mol. weight [g/mol]:	307.38

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.487		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpola	2016.00		NIST Webbook

## Sources

McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369015&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## 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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