

# 2,6-Pyridinedicarboxylic acid, hexadecyl hexyl ester

Inchi:	InChI=1S/C29H49NO4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-25-34-29(32)27-23-2
InchiKey:	PJBXAKJWPVHRFY-UHFFFAOYSA-N
Formula:	C29H49NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)n1
Mol. weight [g/mol]:	475.70

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.09		Crippen Method
logp	8.457		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
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=U368784&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368784&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>

## Legend

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

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