

# 2,6-Pyridinedicarboxylic acid, 2-(2-methoxyethyl)heptyl pentyl ester

Inchi:	InChI=1S/C22H35NO5/c1-4-6-8-11-18(14-16-26-3)17-28-22(25)20-13-10-12-19(23-20)2
InchiKey:	MTLWBSVBBOIFAA-UHFFFAOYSA-N
Formula:	C22H35NO5
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCC(CCCCC)CCOC)n1
Mol. weight [g/mol]:	393.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.01		Crippen Method
logp	4.818		Crippen Method
mcvol	327.810	ml/mol	McGowan Method
rinpola	2737.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
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=U369186&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369186&amp;Units=SI</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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