

# 2,6-Pyridinedicarboxylic acid, 2-ethylhexyl tridecyl ester

Inchi:	InChI=1S/C28H47NO4/c1-4-7-9-10-11-12-13-14-15-16-17-22-32-27(30)25-20-18-21-26(2)
InchiKey:	VCZRNOWKUIASKS-UHFFFAOYSA-N
Formula:	C28H47NO4
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(CC)CCCC)n1
Mol. weight [g/mol]:	461.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.43		Crippen Method
logp	7.923		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
rinsol	3151.00		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=U368276&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368276&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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