

# 2,6-Pyridinedicarboxylic acid, heptyl 3-(2-methoxyethyl)nonyl ester

<b>Inchi:</b>	InChI=1S/C26H43NO5/c1-4-6-8-10-12-19-31-25(28)23-15-13-16-24(27-23)26(29)32-21-
<b>InchiKey:</b>	PRPLEHJBHVEKMJ-UHFFFAOYSA-N
<b>Formula:</b>	C26H43NO5
<b>SMILES:</b>	CCCCCCCOC(=O)c1cccc(C(=O)OCCC(CCCCC)CCOC)n1
<b>Mol. weight [g/mol]:</b>	449.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	6.379		Crippen Method
mcvol	384.170	ml/mol	McGowan Method
rinpola	3078.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369211&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-521-5/2-6-Pyridinedicarboxylic-acid-heptyl-3-2-methoxyethyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-20 02:09:06.460513011 +0000 UTC m=+15868195.381090386.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.