

# 2,6-Pyridinedicarboxylic acid, pentyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C20H31NO4/c1-6-7-8-12-24-18(22)16-10-9-11-17(21-16)19(23)25-14-15(2)13
InchiKey:	TYBMPZKVIKZSASK-UHFFFAOYSA-N
Formula:	C20H31NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1
Mol. weight [g/mol]:	349.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	4.658		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
rinpole	2374.00		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=U368791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368791&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
rinpole:	Non-polar retention indices

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