

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

**Inchi:** InChI=1S/C32H55NO4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-36-30(34)28-29  
**InchiKey:** MUPDLYHSRNWBNP-UHFFFAOYSA-N  
**Formula:** C32H55NO4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC(C)(C)C)n1  
**Mol. weight [g/mol]:** 517.78

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.87		Crippen Method
logp	9.339		Crippen Method
mcvol	462.840	ml/mol	McGowan Method
rinpole	3387.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U368803&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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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