

# 2,6-Pyridinedicarboxylic acid, heptyl 2-octyl ester

Inchi:	InChI=1S/C22H35NO4/c1-4-6-8-10-12-17-26-21(24)19-15-13-16-20(23-19)22(25)27-18(3)
InchiKey:	NJWMVLZSKNXCOF-UHFFFAOYSA-N
Formula:	C22H35NO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OC(C)CCCCC)n1
Mol. weight [g/mol]:	377.52

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.28		Crippen Method
logp	5.724		Crippen Method
mcvol	321.940	ml/mol	McGowan Method
rinsol	2628.00		NIST Webbook

## Sources

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=U368303&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368303&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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