

2,6-Pyridinedicarboxylic acid, hexyl 2-octyl ester

Inchi:	InChI=1S/C21H33NO4/c1-4-6-8-10-13-17(3)26-21(24)19-15-12-14-18(22-19)20(23)25-16
InchiKey:	YSALCJZTUNRWLN-UHFFFAOYSA-N
Formula:	C21H33NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC(C)CCCC)n1
Mol. weight [g/mol]:	363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.86		Crippen Method
logp	5.334		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinsol	2525.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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