

2,6-Pyridinedicarboxylic acid, heptyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C21H33NO4/c1-5-7-8-9-10-15-25-20(23)17-13-11-14-18(22-17)21(24)26-19(12)
InchiKey:	VAJSYITWTBHKDK-UHFFFAOYSA-N
Formula:	C21H33NO4
SMILES:	CCCCCCCOC(=O)c1cccc(C(=O)OC(CCC)C(C)C)n1
Mol. weight [g/mol]:	363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	5.190		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinpola	2457.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369024&Units=SI

Legend

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

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