

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

Inchi:	InChI=1S/C18H27NO4/c1-4-6-7-8-13-22-17(20)15-11-9-12-16(19-15)18(21)23-14(3)10-5
InchiKey:	IHXAHDDFZYWXDL-UHFFFAOYSA-N
Formula:	C18H27NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OC(C)CCC)n1
Mol. weight [g/mol]:	321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.60		Crippen Method
logp	4.164		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinsol	2262.00		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=U368336&Units=SI

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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