

2,6-Pyridinedicarboxylic acid, hexyl neopentyl ester

Inchi:	InChI=1S/C18H27NO4/c1-5-6-7-8-12-22-16(20)14-10-9-11-15(19-14)17(21)23-13-18(2,3
InchiKey:	OTXNNYCPQJWCWRF-UHFFFAOYSA-N
Formula:	C18H27NO4
SMILES:	CCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
Mol. weight [g/mol]:	321.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.022		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
rinsol	2225.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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