

2,6-Pyridinedicarboxylic acid, heptyl isobutyl ester

Inchi:	InChI=1S/C18H27NO4/c1-4-5-6-7-8-12-22-17(20)15-10-9-11-16(19-15)18(21)23-13-14(2
InchiKey:	DVLWEHZNOZOHIW-UHFFFAOYSA-N
Formula:	C18H27NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCC(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
rinpol	2310.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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