

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

Inchi: InChI=1S/C18H27NO4/c1-4-6-7-8-12-22-17(20)15-10-9-11-16(19-15)18(21)23-13-14(3)5
InchiKey: LWZRCWNFLJIVAS-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)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	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369062&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
rinpol: Non-polar retention indices

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