

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

Inchi: InChI=1S/C17H25NO4/c1-4-6-7-11-21-16(19)14-9-8-10-15(18-14)17(20)22-12-13(3)5-2/
InchiKey: VFUOVFOUGMCRBO-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCC(C)CC)n1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.632		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
rinpole	2219.00		NIST Webbook
rinpole	2219.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369060&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
rinpole: Non-polar retention indices

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