

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

Inchi: InChI=1S/C14H19NO4/c1-4-10(3)9-19-14(17)12-8-6-7-11(15-12)13(16)18-5-2/h6-8,10H,
InchiKey: YIJWWMSEVYHWNJ-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCOC(=O)c1cccc(C(=O)OCC(C)CC)n1
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.461		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
rinsol	1926.00		NIST Webbook

Sources

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=U369056&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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