

2,6-Pyridinedicarboxylic acid, 5-methoxy-3-methylpent-2-yl propyl ester

Inchi: InChI=1S/C17H25NO5/c1-5-10-22-16(19)14-7-6-8-15(18-14)17(20)23-13(3)12(2)9-11-21
InchiKey: ZRKBMNFABHGLHO-UHFFFAOYSA-N
Formula: C17H25NO5
SMILES: CCCOC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1
Mol. weight [g/mol]: 323.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.03		Crippen Method
logp	2.866		Crippen Method
mcvol	257.360	ml/mol	McGowan Method
rinpola	2239.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369171&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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
rinpola: Non-polar retention indices

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