

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

Inchi: InChI=1S/C15H21NO4/c1-4-7-11(3)10-20-15(18)13-9-6-8-12(16-13)14(17)19-5-2/h6,8-9,
InchiKey: BIVCIXIIBULAPH-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CCCC(C)COC(=O)c1cccc(C(=O)OCC)n1
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.851		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpole	2015.00		NIST Webbook
rinpole	2015.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369080&Units=SI>

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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