2,6-Pyridinedicarboxylic acid, neopentyl propyl ester

Inchi: InChI=1S/C15H21NO4/c1-5-9-19-13(17)11-7-6-8-12(16-11)14(18)20-10-15(2,3)4/h6-8H,5

InchiKey: HCJPFIFUGUFGFO-UHFFFAOYSA-N

Formula: C15H21NO4

SMILES: CCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)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
rinpol	1925.00		NIST Webbook
rinpol	1925.00		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=U368998&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.