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

Inchi: InChI=1S/C20H31NO5/c1-5-6-7-8-13-25-19(22)17-10-9-11-18(21-17)20(23)26-16(3)15(2

InchiKey: LLIDIZFNXQLIBO-UHFFFAOYSA-N

Formula: C20H31NO5

SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1

Mol. weight [g/mol]: 365.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.28		Crippen Method
logp	4.037		Crippen Method
mcvol	299.630	ml/mol	McGowan Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369175&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.