2,6-Pyridinedicarboxylic acid, butyl phenethyl ester

Inchi: InChI=1S/C19H21NO4/c1-2-3-13-23-18(21)16-10-7-11-17(20-16)19(22)24-14-12-15-8-5-

InchiKey: KSLNZABWRXXCPT-UHFFFAOYSA-N

Formula: C19H21NO4

SMILES: CCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.438		Crippen Method
mcvol	255.910	ml/mol	McGowan Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369224&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.