2,6-Pyridinedicarboxylic acid, pentyl phenethyl ester

Inchi: InChI=1S/C20H23NO4/c1-2-3-7-14-24-19(22)17-11-8-12-18(21-17)20(23)25-15-13-16-9-

InchiKey: KENXGFRBKKDNJD-UHFFFAOYSA-N

Formula: C20H23NO4

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

Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	3.828		Crippen Method
mcvol	270.000	ml/mol	McGowan Method
rinpol	2683.00		NIST Webbook
rinpol	2683.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369225&Units=SI

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

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

rinpol: Non-polar retention indices

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