2,6-Pyridinedicarboxylic acid, 2-methoxyphenyl octyl ester

Inchi: InChI=1S/C22H27NO5/c1-3-4-5-6-7-10-16-27-21(24)17-12-11-13-18(23-17)22(25)28-20-

InchiKey: BWHLFELKXBXTRA-UHFFFAOYSA-N

Formula: C22H27NO5

SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC)n1

Mol. weight [g/mol]: 385.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	4.827		Crippen Method
mcvol	304.050	ml/mol	McGowan Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369220&Units=SI

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.