2,6-Pyridinedicarboxylic acid, 4-bromo-2-methoxybenzyl pentyl ester

Inchi: InChI=1S/C20H22BrNO5/c1-3-4-5-11-26-19(23)16-7-6-8-17(22-16)20(24)27-13-14-9-10-

InchiKey: AVHANJNSCZQHOQ-UHFFFAOYSA-N

Formula: C20H22BrNO5

SMILES: CCCCCOC(=O)c1cccc(C(=O)OCc2ccc(Br)cc2OC)n1

Mol. weight [g/mol]: 436.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	4.557		Crippen Method
mcvol	293.370	ml/mol	McGowan Method
rinpol	3060.00		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=U369168&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