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

Inchi: InChI=1S/C17H16BrNO5/c1-3-23-16(20)13-5-4-6-14(19-13)17(21)24-10-11-7-8-12(18)9-

InchiKey: SVWSOOFMJHVKHH-UHFFFAOYSA-N

Formula: C17H16BrNO5

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

Mol. weight [g/mol]: 394.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	3.386		Crippen Method
mcvol	251.100	ml/mol	McGowan Method
rinpol	2833.00		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=U369167&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