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

Inchi: InChI=1S/C17H17NO5/c1-3-22-16(19)14-5-4-6-15(18-14)17(20)23-11-12-7-9-13(21-2)10

InchiKey: XEWXCXWUVOCANO-UHFFFAOYSA-N

Formula: C17H17NO5

SMILES: CCOC(=O)c1cccc(C(=O)OCc2ccc(OC)cc2)n1

Mol. weight [g/mol]: 315.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.624		Crippen Method
mcvol	233.600	ml/mol	McGowan Method
rinpol	2601.00		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=U369214&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