2,6-Pyridinedicarboxylic acid, ethyl phenethyl ester

Inchi: InChI=1S/C17H17NO4/c1-2-21-16(19)14-9-6-10-15(18-14)17(20)22-12-11-13-7-4-3-5-8-
InchiKey: FZQSXFXHIOPKEI-UHFFFAOYSA-N
Formula: C17H17NO4
SMILES: CCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	2.658		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		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=U369222&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

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