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

Inchi: InChI=1S/C21H25NO5/c1-3-4-5-6-9-15-26-20(23)16-11-10-12-17(22-16)21(24)27-19-14-

InchiKey: AEAMXZAYOYORRA-UHFFFAOYSA-N

Formula: C21H25NO5

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

Mol. weight [g/mol]: 371.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.20		Crippen Method
logp	4.437		Crippen Method
mcvol	289.960	ml/mol	McGowan Method
rinpol	2874.00		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=U369219&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