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

Inchi: InChI=1S/C20H23NO5/c1-3-4-5-8-14-25-19(22)15-10-9-11-16(21-15)20(23)26-18-13-7-6

InchiKey: ZJOQMVFJDUZLTB-UHFFFAOYSA-N

Formula: C20H23NO5

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

Mol. weight [g/mol]: 357.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	4.046		Crippen Method
mcvol	275.870	ml/mol	McGowan Method
rinpol	2778.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369218&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices