

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

Inchi: InChI=1S/C19H21NO5/c1-3-4-7-13-24-18(21)14-9-8-10-15(20-14)19(22)25-17-12-6-5-11
InchiKey: QQVZBIWCUFVZJA-UHFFFAOYSA-N
Formula: C19H21NO5
SMILES: CCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2OC)n1
Mol. weight [g/mol]: 343.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	3.656		Crippen Method
mcvol	261.780	ml/mol	McGowan Method
rinpola	2681.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U369217&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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