

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: CCCCCCOC(=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

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