2,6-Pyridinedicarboxylic acid, diheptyl ester

Inchi: InChI=1S/C21H33NO4/c1-3-5-7-9-11-16-25-20(23)18-14-13-15-19(22-18)21(24)26-17-12
InchiKey: KRMYNURDRUJUKE-UHFFFAOYSA-N
Formula: C21H33NO4
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCCCCCC)n1
Mol. weight [g/mol]: 363.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.75		Crippen Method
logp	5.336		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
rinpol	2643.00		NIST Webbook
rinpol	2643.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369025&Units=SI

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.