2,6-Pyridinedicarboxylic acid, heptyl 3-(2-methoxyethyl)heptyl ester

Inchi: InChI=1S/C24H39NO5/c1-4-6-8-9-10-17-29-23(26)21-13-11-14-22(25-21)24(27)30-19-16
InchiKey: GSHFSZCHYAFOQK-UHFFFAOYSA-N
Formula: C24H39NO5
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCCC(CCCC)CCOC)n1
Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	5.599		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
rinpol	2942.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369115&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