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

Inchi: InChI=1S/C21H33NO5/c1-4-6-9-17(12-15-25-3)13-16-27-21(24)19-11-8-10-18(22-19)20(
InchiKey: KTWISGPAFRWNIE-UHFFFAOYSA-N
Formula: C21H33NO5
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCC(CCCC)CCOC)n1
Mol. weight [g/mol]: 379.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.59		Crippen Method
logp	4.428		Crippen Method
mcvol	313.720	ml/mol	McGowan Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		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=U369112&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.