

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

Inchi: InChI=1S/C21H33NO5/c1-4-6-8-10-17(13-15-25-3)16-27-21(24)19-12-9-11-18(22-19)20
InchiKey: SUNSPOQMAIAZBM-UHFFFAOYSA-N
Formula: C21H33NO5
SMILES: CCCCCC(COC)COC(=O)c1cccc(C(=O)OCCCC)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
rinpola	2642.00		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=U369185&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
rinpola: Non-polar retention indices

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