

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

Inchi: InChI=1S/C29H49NO5/c1-4-6-8-9-10-11-12-13-14-16-22-34-28(31)26-19-17-20-27(30-29)
InchiKey: YPJOIZWXILBDID-UHFFFAOYSA-N
Formula: C29H49NO5
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 491.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	7.549		Crippen Method
mcvol	426.440	ml/mol	McGowan Method
rinsol	3251.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369192&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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