

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

Inchi: InChI=1S/C20H31NO5/c1-4-6-7-9-16(12-14-24-3)15-26-20(23)18-11-8-10-17(21-18)19(2)
InchiKey: AWRLMJLWPNTIBC-UHFFFAOYSA-N
Formula: C20H31NO5
SMILES: CCCCCC(CCOC)COC(=O)c1cccc(C(=O)OCCC)n1
Mol. weight [g/mol]: 365.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	4.038		Crippen Method
mcvol	299.630	ml/mol	McGowan Method
rinpol	2552.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369183&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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
rinpol: Non-polar retention indices

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