

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

Inchi: InChI=1S/C26H43NO5/c1-4-6-8-9-10-11-13-19-31-25(28)23-16-14-17-24(27-23)26(29)30
InchiKey: HTONFYWHYDTAOJ-UHFFFAOYSA-N
Formula: C26H43NO5
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 449.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.68		Crippen Method
logp	6.379		Crippen Method
mcvol	384.170	ml/mol	McGowan Method
rinpola	3068.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369190&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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