

2,6-Pyridinedicarboxylic acid, 3-(2-methoxyethyl)nonyl octyl ester

Inchi: InChI=1S/C27H45NO5/c1-4-6-8-10-11-13-20-32-26(29)24-16-14-17-25(28-24)27(30)33-2
InchiKey: MMJXYOZWCXYJZKL-UHFFFAOYSA-N
Formula: C27H45NO5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 463.65

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.10 | | Crippen Method |
| logp | 6.769 | | Crippen Method |
| mcvol | 398.260 | ml/mol | McGowan Method |
| rinpol | 3137.00 | | NIST Webbook |
| rinpol | 3137.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U369212&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

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