

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

Inchi: InChI=1S/C23H37NO5/c1-5-6-7-8-10-19(13-15-27-4)14-16-28-22(25)20-11-9-12-21(24-2)
InchiKey: HGAKBZYQASXDOR-UHFFFAOYSA-N
Formula: C23H37NO5
SMILES: CCCCCC(CCOC)CCOC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]: 407.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	5.064		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
rinsol	2795.00		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=U369207&Units=SI>

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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