

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

Inchi: InChI=1S/C25H41NO5/c1-4-6-8-10-13-21(16-19-29-3)17-20-31-25(28)23-15-12-14-22(20)
InchiKey: QFQZMHBTRMPCPT-UHFFFAOYSA-N
Formula: C25H41NO5
SMILES: CCCCCOC(=O)c1cccc(C(=O)OCCC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 435.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.27		Crippen Method
logp	5.989		Crippen Method
mcvol	370.080	ml/mol	McGowan Method
rinpole	3005.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369210&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
rinpole: Non-polar retention indices

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