

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

Inchi: InChI=1S/C23H37NO5/c1-4-6-8-9-16-28-22(25)20-12-10-13-21(24-20)23(26)29-18-15-19
InchiKey: ZBFAWFQEZJNUAG-UHFFFAOYSA-N
Formula: C23H37NO5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCCC(CCCC)CCOC)n1
Mol. weight [g/mol]: 407.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	5.208		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
rinpola	2857.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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=U369114&Units=SI>

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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