

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

Inchi: InChI=1S/C24H39NO5/c1-4-6-8-9-11-17-29-23(26)21-14-12-15-22(25-21)24(27)30-19-20
InchiKey: DKOGNVMTSZOSEX-UHFFFAOYSA-N
Formula: C24H39NO5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	5.599		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
rinpol	2918.00		NIST Webbook

Sources

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=U369188&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/32-980-8/2-6-Pyridinedicarboxylic-acid-heptyl-2-2-methoxyethyl-heptyl-ester.pdf>

Generated by Cheméo on 2025-12-05 15:56:21.932974698 +0000 UTC m=+4698379.463015359.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.