

2,6-Pyridinedicarboxylic acid, hexyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C24H39NO5/c1-4-6-8-10-14-20(15-13-18-28-3)30-24(27)22-17-12-16-21(25-23)1
InchiKey: MXYWWINIQZFMLM-UHFFFAOYSA-N
Formula: C24H39NO5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OC(CCCCC)CCOC)n1
Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	5.741		Crippen Method
mcvol	355.990	ml/mol	McGowan Method
rinpol	2859.00		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=U369247&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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