

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

Inchi: InChI=1S/C25H41NO5/c1-4-6-8-9-10-12-18-30-24(27)22-15-13-16-23(26-22)25(28)31-20
InchiKey: PWNWUJHSBGWQGD-UHFFFAOYSA-N
Formula: C25H41NO5
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCC(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
rinsol	2994.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369189&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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