

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

Inchi: InChI=1S/C22H35NO5/c1-4-6-8-9-12-18(13-11-16-26-3)28-22(25)20-15-10-14-19(23-20)
InchiKey: ONKQZHJCBNZCIU-UHFFFAOYSA-N
Formula: C22H35NO5
SMILES: CCCCCC(CCCOC)OC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]: 393.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	4.961		Crippen Method
mcvol	327.810	ml/mol	McGowan Method
rinpola	2625.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U369245&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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
rinpola: Non-polar retention indices

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