

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

Inchi:	InChI=1S/C26H43NO5/c1-4-6-8-10-11-13-21-31-25(28)23-18-14-19-24(27-23)26(29)32-2
InchiKey:	BDTFYJJXXNZXOA-UHFFFAOYSA-N
Formula:	C26H43NO5
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OC(CCCCC)CCCOC)n1
Mol. weight [g/mol]:	449.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	6.521		Crippen Method
mcvol	384.170	ml/mol	McGowan Method
rinpola	3016.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369249&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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