

2,6-Pyridinedicarboxylic acid, 5-methoxy-3-methylpent-2-yl tridecyl ester

Inchi:	InChI=1S/C27H45NO5/c1-5-6-7-8-9-10-11-12-13-14-15-20-32-26(29)24-17-16-18-25(28)
InchiKey:	HDCDYKNLHVPRJQ-UHFFFAOYSA-N
Formula:	C27H45NO5
SMILES:	CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OC(C)C(C)CCOC)n1
Mol. weight [g/mol]:	463.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.21		Crippen Method
logp	6.767		Crippen Method
mcvol	398.260	ml/mol	McGowan Method
rinsol	3134.00		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=U369179&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
rinsol:	Non-polar retention indices

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