

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

Inchi:	InChI=1S/C19H29NO5/c1-4-6-7-9-15(12-13-23-3)14-25-19(22)17-11-8-10-16(20-17)18(2
InchiKey:	YMTXBWUWLPOWKQ-UHFFFAOYSA-N
Formula:	C19H29NO5
SMILES:	CCCCC(CCOC)COC(=O)c1cccc(C(=O)OCC)n1
Mol. weight [g/mol]:	351.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.75		Crippen Method
logp	3.648		Crippen Method
mcvol	285.540	ml/mol	McGowan Method
rinpola	2469.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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