

2,6-Pyridinedicarboxylic acid, butyl 3-(2-methoxyethyl)nonyl ester

Inchi:	InChI=1S/C23H37NO5/c1-4-6-8-9-11-19(14-17-27-3)15-18-29-23(26)21-13-10-12-20(24
InchiKey:	UNEIIRNGIPLSJR-UHFFFAOYSA-N
Formula:	C23H37NO5
SMILES:	CCCCCCC(CCOC)CCOC(=O)c1cccc(C(=O)OCCCC)n1
Mol. weight [g/mol]:	407.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.43		Crippen Method
logp	5.208		Crippen Method
mcvol	341.900	ml/mol	McGowan Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369208&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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