

2,6-Pyridinedicarboxylic acid, octyl phenethyl ester

Inchi:	InChI=1S/C23H29NO4/c1-2-3-4-5-6-10-17-27-22(25)20-14-11-15-21(24-20)23(26)28-18
InchiKey:	YDZUQTIQGBFEJQ-UHFFFAOYSA-N
Formula:	C23H29NO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1
Mol. weight [g/mol]:	383.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.69		Crippen Method
logp	4.998		Crippen Method
mcvol	312.270	ml/mol	McGowan Method
rinsol	2966.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinsol:	Non-polar retention indices

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