

2,6-Pyridinedicarboxylic acid, butyl 2-methylbutyl ester

Inchi:	InChI=1S/C16H23NO4/c1-4-6-10-20-15(18)13-8-7-9-14(17-13)16(19)21-11-12(3)5-2/h7-9
InchiKey:	PAATVMUOMBFSQT-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCC(C)CC)n1
Mol. weight [g/mol]:	293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.41		Crippen Method
logp	3.241		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpola	2114.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369059&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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