

2,6-Pyridinedicarboxylic acid, isobutyl neopentyl ester

Inchi:	InChI=1S/C16H23NO4/c1-11(2)9-20-14(18)12-7-6-8-13(17-12)15(19)21-10-16(3,4)5/h6-8
InchiKey:	VSSCWKWPZDMWJX-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CC(C)COC(=O)c1cccc(C(=O)OCC(C)(C)C)n1
Mol. weight [g/mol]:	293.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.17		Crippen Method
logp	3.097		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
rinpole	1979.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U368999&Units=SI

Legend

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

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