

2,6-Pyridinedicarboxylic acid, butyl isobutyl ester

Inchi:	InChI=1S/C15H21NO4/c1-4-5-9-19-14(17)12-7-6-8-13(16-12)15(18)20-10-11(2)3/h6-8,1
InchiKey:	VNQVWTAZGXOWHJ-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCC(C)C)n1
Mol. weight [g/mol]:	279.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.851		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368850&Units=SI
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

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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