

2,6-Pyridinedicarboxylic acid, butyl 3-methylbutyl ester

Inchi: InChI=1S/C16H23NO4/c1-4-5-10-20-15(18)13-7-6-8-14(17-13)16(19)21-11-9-12(2)3/h6-
InchiKey: KNFLELUCUMUTDH-UHFFFAOYSA-N
Formula: C16H23NO4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCC(C)C)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
rinpole	2123.00		NIST Webbook
rinpole	2123.00		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=U368315&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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