2-(2,2-Dimethylpentoxy)-3-methyl-6-(n-pentyl) pyrazine

Inchi: InChI=1S/C17H30N2O/c1-6-8-9-10-15-12-18-14(3)16(19-15)20-13-17(4,5)11-7-2/h12H,6

InchiKey: RQHMRSCTXRPRLH-UHFFFAOYSA-N

Formula: C17H30N2O

SMILES: CCCCCc1cnc(C)c(OCC(C)(C)CCC)n1

Mol. weight [g/mol]: 278.43

CAS: 116668-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.93		Crippen Method
logp	4.723		Crippen Method
mcvol	252.460	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116668941&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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