2-(2,2,4-Trimethylpentoxy)-3-(n-pentyl) pyrazine

Inchi: InChI=1S/C17H30N2O/c1-6-7-8-9-15-16(19-11-10-18-15)20-13-17(4,5)12-14(2)3/h10-11

InchiKey: WBRJSGNTCBKXBR-UHFFFAOYSA-N

Formula: C17H30N2O

SMILES: CCCCCc1nccnc1OCC(C)(C)CC(C)C

Mol. weight [g/mol]: 278.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	4.660		Crippen Method
mcvol	252.460	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003302&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume