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

Inchi: InChI=1S/C23H42N2O/c1-6-9-11-12-14-15-20-18-24-21(16-13-10-7-2)22(25-20)26-19-23

InchiKey: WJWWWDDDILISTJ-UHFFFAOYSA-N

Formula: C23H42N2O

SMILES: CCCCCCCc1cnc(CCCCC)c(OCC(C)(C)CCC)n1

Mol. weight [g/mol]: 362.59

CAS: 3049-56-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	6.927		Crippen Method
mcvol	337.000	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3049567&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