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

Inchi: InChI=1S/C19H34N2O/c1-6-8-9-10-11-12-17-14-20-16(3)18(21-17)22-15-19(4,5)13-7-2/h

InchiKey: FSHSCUJFVBMKHO-UHFFFAOYSA-N

Formula: C19H34N2O

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

Mol. weight [g/mol]: 306.49

CAS: 116660-34-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.503		Crippen Method
mcvol	280.640	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=C116660345&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume