2-(2,2,4-Trimethylpentoxy)-3,6-dimethyl pyrazine

Inchi: InChI=1S/C14H24N2O/c1-10(2)7-14(5,6)9-17-13-12(4)15-8-11(3)16-13/h8,10H,7,9H2,1-

InchiKey: HWVHYMQSPCNBIT-UHFFFAOYSA-N

Formula: C14H24N2O

SMILES: Cc1cnc(C)c(OCC(C)(C)CC(C)C)n1

Mol. weight [g/mol]: 236.35

CAS: 116660-26-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.545		Crippen Method
mcvol	210.190	ml/mol	McGowan Method

Sources

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=C116660265&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume