2-(2,2-Dimethylpentoxy)-3-methyl pyrazine

Inchi: InChI=1S/C12H20N2O/c1-5-6-12(3,4)9-15-11-10(2)13-7-8-14-11/h7-8H,5-6,9H2,1-4H3
InchiKey: YUGAMTAQKFTTIT-UHFFFAOYSA-N
Formula: C12H20N2O
SMILES: CCCC(C)(C)COc1nccnc1C
Mol. weight [g/mol]: 208.30
CAS: 116660-28-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	2.990		Crippen Method
mcvol	182.010	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660287&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