2-(2,2-Dimethylpentoxy)-3,6-dimethyl pyrazine

Inchi: InChI=1S/C13H22N2O/c1-6-7-13(4,5)9-16-12-11(3)14-8-10(2)15-12/h8H,6-7,9H2,1-5H3
InchiKey: DSEGKGZERLGYFB-UHFFFAOYSA-N
Formula: C13H22N2O
SMILES: CCCC(C)(C)COc1nc(C)cnc1C
Mol. weight [g/mol]: 222.33
CAS: 116660-21-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.299		Crippen Method
mcvol	196.100	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660210&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume