# 2-(2,2,4-Trimethylpentoxy)-3-methyl pyrazine

**Inchi:** InChI=1S/C13H22N2O/c1-10(2)8-13(4,5)9-16-12-11(3)14-6-7-15-12/h6-7,10H,8-9H2,1-5
**InchiKey:** MABUKNLWUYRSSQ-UHFFFAOYSA-N
**Formula:** C13H22N2O
**SMILES:** Cc1nccnc1OCC(C)(C)CC(C)C
**Mol. weight [g/mol]:** 222.33
**CAS:** 116659-77-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.05 | | Crippen Method |
| logp | 3.236 | | 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=C116659779&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