

2-(1-Hydroxy-1-methylethyl)-5-(1-methylethyl)pyrazine

Inchi: InChI=1S/C10H16N2O/c1-7(2)8-5-12-9(6-11-8)10(3,4)13/h5-7,13H,1-4H3
InchiKey: SEQOBFCOIPROTR-UHFFFAOYSA-N
Formula: C10H16N2O
SMILES: CC(C)c1cnc(C(C)(C)O)cn1
Mol. weight [g/mol]: 180.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -2.84 | | Crippen Method |
| logp | 1.827 | | Crippen Method |
| mcvol | 153.830 | ml/mol | McGowan Method |
| rinpol | 1326.00 | | NIST Webbook |
| rinpol | 1326.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R412805&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
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/39-698-5/2-1-Hydroxy-1-methylethyl-5-1-methylethyl-pyrazine.pdf>

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