

# Pyrazine, 2-[5-(hydroxymethyl)furfuryl]-3,5-dimethyl

**Other names:** 2-(2-(5-(hydroxymethyl)furfuryl))-3,5-dimethylpyrazine

**Inchi:** InChI=1S/C12H14N2O2/c1-8-6-13-12(9(2)14-8)5-10-3-4-11(7-15)16-10/h3-4,6,15H,5,7H

**InchiKey:** JGXGKXSOGRRHHM-UHFFFAOYSA-N

**Formula:** C12H14N2O2

**SMILES:** Cc1cnc(Cc2ccc(CO)o2)c(C)n1

**Mol. weight [g/mol]:** 218.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.93		Crippen Method
logp	1.770		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
rinpol	1702.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1702.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R87928&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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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