

Pyrazine, 2-[5-(hydroxymethyl)furfuryl]-3,6-dimethyl

Inchi: InChI=1S/C12H14N2O2/c1-8-6-13-9(2)12(14-8)5-10-3-4-11(7-15)16-10/h3-4,6,15H,5,7H
InchiKey: DUILMNODMXLXKM-UHFFFAOYSA-N
Formula: C12H14N2O2
SMILES: Cc1cnc(C)c(Cc2ccc(CO)o2)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	1767.00		NIST Webbook
rinpol	1767.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R87932&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/20-081-9/Pyrazine-2-5-hydroxymethyl-furfuryl-3-6-dimethyl.pdf>

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