

Pyrazine, 2-(2-furfuryl)-3,5-dimethyl

Other names: 3-(2-furfuryl)-2,6-dimethylpyrazine
Inchi: InChI=1S/C11H12N2O/c1-8-7-12-11(9(2)13-8)6-10-4-3-5-14-10/h3-5,7H,6H2,1-2H3
InchiKey: AYHLQEAYCNZHDY-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: Cc1cnc(Cc2ccco2)c(C)n1
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.79		Crippen Method
logp	2.277		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1418.00		NIST Webbook
rinpol	1417.00		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=R87843&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/28-986-7/Pyrazine-2-2-furfuryl-3-5-dimethyl.pdf>

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