

2-(2-furfuryl)pyrazine

Other names: Pyrazine, 2-(2-furfuryl)
Inchi: InChI=1S/C9H8N2O/c1-2-9(12-5-1)6-8-7-10-3-4-11-8/h1-5,7H,6H2
InchiKey: RLPOAXAHNABIKV-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: c1coc(Cc2cnccn2)c1
Mol. weight [g/mol]: 160.17

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.84 | | Crippen Method |
| logp | 1.660 | | Crippen Method |
| mcvol | 120.280 | ml/mol | McGowan Method |
| rinpol | 1279.00 | | NIST Webbook |
| rinpol | 1279.00 | | NIST Webbook |
| rinpol | 1279.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R87839&Units=SI>

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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