

2-Methyl-5-isopropenylfuran

Inchi: InChI=1S/C8H10O/c1-6(2)8-5-4-7(3)9-8/h4-5H,1H2,2-3H3
InchiKey: NNTUPAINNBMOFI-UHFFFAOYSA-N
Formula: C8H10O
SMILES: C=C(C)c1ccc(C)o1
Mol. weight [g/mol]: 122.16

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.92 | | Crippen Method |
| logp | 2.621 | | Crippen Method |
| mcvol | 105.690 | ml/mol | McGowan Method |
| rinpol | 937.00 | | NIST Webbook |
| rinpol | 932.00 | | NIST Webbook |
| rinpol | 932.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |
| rinpol | 933.00 | | NIST Webbook |

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R625462&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

Latest version available from:

<https://www.chemeo.com/cid/73-266-6/2-Methyl-5-isopropenylfuran.pdf>

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