# 1-Propanone, 1-(5-methyl-2-furanyl)-

| | |
|---|---|
| **Other names:** | 2-Methyl-5-propionylfuran |
| | 1-Propanone, 1-(5-methyl-2-furyl)- |
| | 5-Methyl-2-propionylfuran |
| | 1-(5-Methyl-2-furyl)-1-propanone |
| | 1-(5-Methyl-2-furanyl)-1-propanone |
| | Furan, 2-methyl-5-propionyl |
| | Furan, 5-methyl-2-propionyl |
| | 5-Methyl-5-propionylfuran |
| | 1-(5-methyl-2-furyl)propan-1-one |
| **Inchi:** | InChI=1S/C8H10O2/c1-3-7(9)8-5-4-6(2)10-8/h4-5H,3H2,1-2H3 |
| **InchiKey:** | BXLPZYAVKVFXEO-UHFFFAOYSA-N |
| **Formula:** | C8H10O2 |
| **SMILES:** | CCC(=O)c1ccc(C)o1 |
| **Mol. weight [g/mol]:** | 138.16 |
| **CAS:** | 10599-69-6 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -6.76 | | Crippen Method |
| logp | 2.181 | | Crippen Method |
| mcvol | 111.560 | ml/mol | McGowan Method |
| rinpol | 1099.00 | | NIST Webbook |
| rinpol | 1151.00 | | NIST Webbook |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1106.00 | | NIST Webbook |
| ripol | 1686.00 | | NIST Webbook |
| ripol | 1686.00 | | NIST Webbook |
| ripol | 1663.00 | | NIST Webbook |
| ripol | 1669.00 | | NIST Webbook |
| ripol | 1670.00 | | NIST Webbook |
| ripol | 1670.00 | | NIST Webbook |
| ripol | 1670.00 | | NIST Webbook |
| ripol | 1700.00 | | NIST Webbook |
| ripol | 1670.00 | | NIST Webbook |
| ripol | 1672.00 | | 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=C10599696&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |