# 2-Formyl-4,5-dimethyl-pyrrole

**Inchi:** InChI=1S/C7H9NO/c1-5-3-7(4-9)8-6(5)2/h3-4,8H,1-2H3
**InchiKey:** SCJGLQUCTCAPAB-UHFFFAOYSA-N
**Formula:** C7H9NO
**SMILES:** Cc1cc(C=O)[nH]c1C
**Mol. weight [g/mol]:** 123.15
**CAS:** 53700-95-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -1.88 | | Crippen Method |
| logp | 0.962 | | Crippen Method |
| mcvol | 101.580 | ml/mol | McGowan Method |
| rinpol | 1168.00 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C53700951&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.