

# 4,5-Dimethyl-2-isopropylloxazole

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Oxazole, 4,5-dimethyl-2-(1-methylethyl)-<br>2-iso-Propyl-4,5-dimethyloxazole<br>Oxazole, 2-isopropyl-4,5-dimethyl |
| <b>Inchi:</b>               | InChI=1S/C8H13NO/c1-5(2)8-9-6(3)7(4)10-8/h5H,1-4H3  |
| <b>InchiKey:</b>            | OHMVVHYBMWXHSY-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C8H13NO   |
| <b>SMILES:</b>              | Cc1nc(C(C)C)oc1C  |
| <b>Mol. weight [g/mol]:</b> | 139.19  |
| <b>CAS:</b>                 | 19519-45-0  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.11   |        | Crippen Method |
| logp          | 2.415   |        | Crippen Method |
| mcvol         | 119.970 | ml/mol | McGowan Method |
| rinpol        | 938.00  |        | NIST Webbook   |
| rinpol        | 960.00  |        | NIST Webbook   |
| ripol         | 1261.00 |        | NIST Webbook   |
| ripol         | 1260.00 |        | NIST Webbook   |
| ripol         | 1261.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C19519450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19519450&amp;Units=SI</a> |

## 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

Latest version available from:

<https://www.cheméo.com/cid/18-484-5/4-5-Dimethyl-2-isopropylloxazole.pdf>

Generated by Cheméo on 2024-04-27 03:55:24.848356122 +0000 UTC m=+16479373.768933438.

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