

# 4-Isobutylpyridine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Pyridine, 4-(2-methylpropyl)                              |
| <b>Inchi:</b>               | InChI=1S/C9H13N/c1-8(2)7-9-3-5-10-6-4-9/h3-6,8H,7H2,1-2H3 |
| <b>InchiKey:</b>            | WACPXLKEEAMYCH-UHFFFAOYSA-N                               |
| <b>Formula:</b>             | C9H13N  |
| <b>SMILES:</b>              | CC(C)Cc1ccncc1  |
| <b>Mol. weight [g/mol]:</b> | 135.21  |
| <b>CAS:</b>                 | 4810-79-1   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.64   |        | Crippen Method |
| logp          | 2.280   |        | Crippen Method |
| mcvol         | 123.890 | ml/mol | McGowan Method |
| rinpol        | 1105.00 |        | NIST Webbook   |
| rinpol        | 1122.00 |        | NIST Webbook   |
| rinpol        | 1105.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4810791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4810791&amp;Units=SI</a> |
| <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>                       |

## Legend

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

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