

# Benzene, 1-azido-4-methyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Toluene, p-azido-<br>p-Azidotoluene<br>p-Tolyl azide<br>1-Azido-4-methylbenzene<br>4-Methylphenyl azide |
| <b>Inchi:</b>               | InChI=1S/C7H7N3/c1-6-2-4-7(5-3-6)9-10-8/h2-5H,1H3   |
| <b>InchiKey:</b>            | YVXDRCDGBCOJHX-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C7H7N3  |
| <b>SMILES:</b>              | <chem>Cc1ccc(N=[N+]=[N-])cc1</chem>   |
| <b>Mol. weight [g/mol]:</b> | 133.15  |
| <b>CAS:</b>                 | 2101-86-2   |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.60   |        | Crippen Method |
| logp          | 2.937   |        | Crippen Method |
| mcpvol        | 107.070 | ml/mol | McGowan Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 353.00 | K    | 1.30           | 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=C2101862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2101862&amp;Units=SI</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>tbrp:</b>    | Boiling point at reduced pressure   |

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