

# p-Butoxytoluene

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | n-Butyl p-tolyl ether<br>4-(n-Butoxy)toluene<br>Benzene, 1-butoxy-4-methyl-<br>butyl p-tolyl ether |
| <b>Inchi:</b>               | InChI=1S/C11H16O/c1-3-4-9-12-11-7-5-10(2)6-8-11/h5-8H,3-4,9H2,1-2H3                                |
| <b>InchiKey:</b>            | AGARRLZBNOJWLG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C11H16O  |
| <b>SMILES:</b>              | CCCCOc1ccc(C)cc1   |
| <b>Mol. weight [g/mol]:</b> | 164.24   |
| <b>CAS:</b>                 | 10519-06-9   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 39.52   | kJ/mol               | Joback Method  |
| hf            | -177.53 | kJ/mol               | Joback Method  |
| hfus          | 19.09   | kJ/mol               | Joback Method  |
| hvap          | 45.43   | kJ/mol               | Joback Method  |
| log10ws       | -3.32   |                      | Crippen Method |
| logp          | 3.174   |                      | Crippen Method |
| mcvol         | 147.960 | ml/mol               | McGowan Method |
| pc            | 2563.69 | kPa                  | Joback Method  |
| tb            | 505.16  | K                    | Joback Method  |
| tc            | 706.73  | K                    | Joback Method  |
| tf            | 274.90  | K                    | Joback Method  |
| vc            | 0.561   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 326.06 | J/mol×K | 505.16          | Joback Method |
| cpg           | 395.24 | J/mol×K | 673.13          | Joback Method |
| cpg           | 382.80 | J/mol×K | 639.54          | Joback Method |
| cpg           | 369.68 | J/mol×K | 605.94          | Joback Method |
| cpg           | 355.85 | J/mol×K | 572.35          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 341.32    | J/mol×K | 538.75 | Joback Method |
| cpg   | 407.02    | J/mol×K | 706.73 | Joback Method |
| dvisc | 0.0001779 | Paxs    | 505.16 | Joback Method |
| dvisc | 0.0002253 | Paxs    | 466.78 | Joback Method |
| dvisc | 0.0002975 | Paxs    | 428.41 | Joback Method |
| dvisc | 0.0004152 | Paxs    | 390.03 | Joback Method |
| dvisc | 0.0006230 | Paxs    | 351.65 | Joback Method |
| dvisc | 0.0010326 | Paxs    | 313.28 | Joback Method |
| dvisc | 0.0019708 | Paxs    | 274.90 | Joback Method |

## 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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C10519069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10519069&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <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>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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