

Benzenemethanol, «alpha»,4-dimethyl-

Other names: Benzyl alcohol, p,«alpha»-dimethyl-p-Tolylmethylcarbinol p,«alpha»-Dimethylbenzyl alcohol Bilagen Galinex Methyl-p-tolylcarbinol Norbilan Tomobil 1-(p-Methylphenyl)ethanol 1-(4-Methylphenyl)ethanol 1-(4-Tolyl)ethanol 1-p-Tolyl-1-ethanol 1-p-Tolylethanol 4-(«alpha»-Hydroxyethyl)toluene 4-Methyl-«alpha»-phenethyl alcohol «alpha»,4-Dimethylbenzyl alcohol «alpha»,4-Dimethylbenzenemethanol Ethanol, 1-(p-tolyl)- 4-Methylphenylmethylcarbinol Ethanol, 1-(4-methylphenyl) (.+/-.)-p,«alpha»-Dimethylbenzyl alcohol Methyl p-methylphenyl carbinol NSC 41714

Inchi: InChI=1S/C9H12O/c1-7-3-5-9(6-4-7)8(2)10/h3-6,8,10H,1-2H3

InchiKey: JESIHYIJKKUWIS-UHFFFAOYSA-N

Formula: C9H12O

SMILES: Cc1ccc(C(C)O)cc1

Mol. weight [g/mol]: 136.19

CAS: 5788-09-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|---------------|
| gf | -11.58 | kJ/mol | Joback Method |
| hf | -161.54 | kJ/mol | Joback Method |
| hfus | 13.28 | kJ/mol | Joback Method |
| hvap | 54.86 | kJ/mol | Joback Method |

| | | | |
|---------|---------|---------|----------------|
| log10ws | -2.47 | | Crippen Method |
| logp | 2.048 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3602.88 | kPa | Joback Method |
| tb | 528.72 | K | Joback Method |
| tc | 728.91 | K | Joback Method |
| tf | 275.95 | K | Joback Method |
| vc | 0.445 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 266.77 | J/mol×K | 528.72 | Joback Method |
| cpg | 278.42 | J/mol×K | 562.08 | Joback Method |
| cpg | 289.43 | J/mol×K | 595.45 | Joback Method |
| cpg | 299.83 | J/mol×K | 628.81 | Joback Method |
| cpg | 309.65 | J/mol×K | 662.18 | Joback Method |
| cpg | 318.90 | J/mol×K | 695.54 | Joback Method |
| cpg | 327.61 | J/mol×K | 728.91 | Joback Method |
| dvisc | 0.0169073 | Paxs | 275.95 | Joback Method |
| dvisc | 0.0042083 | Paxs | 318.08 | Joback Method |
| dvisc | 0.0014502 | Paxs | 360.21 | Joback Method |
| dvisc | 0.0006246 | Paxs | 402.34 | Joback Method |
| dvisc | 0.0003156 | Paxs | 444.46 | Joback Method |
| dvisc | 0.0001795 | Paxs | 486.59 | Joback Method |
| dvisc | 0.0001117 | Paxs | 528.72 | Joback Method |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5788090&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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