

Benzeneethanol, 3-methyl-

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|-----------------------------|---|
| Other names: | Phenethyl alcohol, m-methyl- m-Methylphenethyl alcohol 2-m-Tolylethanol |
| Inchi: | InChI=1S/C9H12O/c1-8-3-2-4-9(7-8)5-6-10/h2-4,7,10H,5-6H2,1H3 |
| InchiKey: | KWHVBVJDKLSOTB-UHFFFAOYSA-N |
| Formula: | C9H12O |
| SMILES: | Cc1cccc(CCO)c1 |
| Mol. weight [g/mol]: | 136.19 |
| CAS: | 1875-89-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -9.14 | kJ/mol | Joback Method |
| hf | -156.26 | kJ/mol | Joback Method |
| hfus | 16.81 | kJ/mol | Joback Method |
| hvap | 55.25 | kJ/mol | Joback Method |
| log10ws | -2.01 | | Crippen Method |
| logp | 1.530 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3568.53 | kPa | Joback Method |
| tb | 515.70 | K | NIST Webbook |
| tc | 725.15 | K | Joback Method |
| tf | 290.95 | K | Joback Method |
| vc | 0.451 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 266.45 | J/mol×K | 529.16 | Joback Method |
| cpg | 317.36 | J/mol×K | 692.49 | Joback Method |
| cpg | 308.29 | J/mol×K | 659.82 | Joback Method |
| cpg | 298.68 | J/mol×K | 627.16 | Joback Method |
| cpg | 288.52 | J/mol×K | 594.49 | Joback Method |
| cpg | 277.78 | J/mol×K | 561.83 | Joback Method |

| | | | | |
|-------|-----------|---------|--------|---------------|
| cpg | 325.92 | J/mol×K | 725.15 | Joback Method |
| dvisc | 0.0001184 | Paxs | 529.16 | Joback Method |
| dvisc | 0.0001835 | Paxs | 489.46 | Joback Method |
| dvisc | 0.0003073 | Paxs | 449.76 | Joback Method |
| dvisc | 0.0005687 | Paxs | 410.05 | Joback Method |
| dvisc | 0.0012010 | Paxs | 370.35 | Joback Method |
| dvisc | 0.0030353 | Paxs | 330.65 | Joback Method |
| dvisc | 0.0098792 | Paxs | 290.95 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1875894&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

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 |

Latest version available from:

<https://www.chemeo.com/cid/63-641-0/Benzeneethanol-3-methyl.pdf>

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