

# Benzenemethanol, «alpha»-(ethoxymethyl)-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | «alpha»-(Ethoxymethyl)benzyl alcohol                                  |
| <b>Inchi:</b>               | InChI=1S/C10H14O2/c1-2-12-8-10(11)9-6-4-3-5-7-9/h3-7,10-11H,2,8H2,1H3 |
| <b>InchiKey:</b>            | XSBXONDDSWGIMG-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H14O2  |
| <b>SMILES:</b>              | CCOCC(O)c1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 166.22  |
| <b>CAS:</b>                 | 22383-53-5  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -98.53  | kJ/mol               | Joback Method  |
| hf            | -302.93 | kJ/mol               | Joback Method  |
| hfus          | 17.45   | kJ/mol               | Joback Method  |
| hvap          | 58.83   | kJ/mol               | Joback Method  |
| log10ws       | -1.92   |                      | Crippen Method |
| logp          | 1.756   |                      | Crippen Method |
| mcvol         | 139.740 | ml/mol               | McGowan Method |
| pc            | 3213.68 | kPa                  | Joback Method  |
| tb            | 569.04  | K                    | Joback Method  |
| tc            | 763.83  | K                    | Joback Method  |
| tf            | 296.93  | K                    | Joback Method  |
| vc            | 0.518   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 336.30    | J/mol×K | 569.04          | Joback Method |
| cpg           | 348.87    | J/mol×K | 601.51          | Joback Method |
| cpg           | 360.77    | J/mol×K | 633.97          | Joback Method |
| cpg           | 372.02    | J/mol×K | 666.44          | Joback Method |
| cpg           | 382.64    | J/mol×K | 698.90          | Joback Method |
| cpg           | 392.65    | J/mol×K | 731.37          | Joback Method |
| cpg           | 402.07    | J/mol×K | 763.83          | Joback Method |
| dvisc         | 0.0122682 | Paxs    | 296.93          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0029883 | Paxs | 342.28 | Joback Method |
| dvisc | 0.0010130 | Paxs | 387.63 | Joback Method |
| dvisc | 0.0004307 | Paxs | 432.99 | Joback Method |
| dvisc | 0.0002154 | Paxs | 478.34 | Joback Method |
| dvisc | 0.0001214 | Paxs | 523.69 | Joback Method |
| dvisc | 0.0000750 | Paxs | 569.04 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=C22383535&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22383535&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>   |

## 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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