

# Benzene, 1,1'-(1,2-ethanediyl)bis[2-methyl-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Benzene, 1,1'-(1,2-ethanediyl)bis*2-methyl-                                       |
| <b>Inchi:</b>               | InChI=1S/C16H18/c1-13-7-3-5-9-15(13)11-12-16-10-6-4-8-14(16)2/h3-10H,11-12H2,1-2H |
| <b>InchiKey:</b>            | QFEPNMCDSBNJDB-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C16H18  |
| <b>SMILES:</b>              | Cc1cccc1CCc1cccc1C  |
| <b>Mol. weight [g/mol]:</b> | 210.31  |
| <b>CAS:</b>                 | 952-80-7  |

## Physical Properties

| Property code | Value           | Unit    | Source         |
|---------------|-----------------|---------|----------------|
| chs           | -8828.60 ± 2.00 | kJ/mol  | NIST Webbook   |
| gf            | 289.40          | kJ/mol  | Joback Method  |
| hf            | 76.55           | kJ/mol  | Joback Method  |
| hfus          | 24.50           | kJ/mol  | Joback Method  |
| hvap          | 57.09           | kJ/mol  | Joback Method  |
| log10ws       | -4.84           |         | Crippen Method |
| logp          | 4.089           |         | Crippen Method |
| mcvol         | 188.780         | ml/mol  | McGowan Method |
| pc            | 2220.80         | kPa     | Joback Method  |
| tb            | 628.80          | K       | Joback Method  |
| tc            | 860.73          | K       | Joback Method  |
| tf            | 340.00 ± 2.00   | K       | NIST Webbook   |
| tf            | 330.00 ± 4.00   | K       | NIST Webbook   |
| vc            | 0.716           | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 471.73 | J/molxK | 628.80          | Joback Method |
| cpg           | 489.89 | J/molxK | 667.45          | Joback Method |
| cpg           | 506.82 | J/molxK | 706.11          | Joback Method |
| cpg           | 522.58 | J/molxK | 744.76          | Joback Method |
| cpg           | 537.22 | J/molxK | 783.42          | Joback Method |
| cpg           | 550.82 | J/molxK | 822.07          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 563.43    | J/molxK | 860.73 | Joback Method |
| dvisc | 0.0014473 | Paxs    | 347.96 | Joback Method |
| dvisc | 0.0007888 | Paxs    | 394.77 | Joback Method |
| dvisc | 0.0004889 | Paxs    | 441.57 | Joback Method |
| dvisc | 0.0003321 | Paxs    | 488.38 | Joback Method |
| dvisc | 0.0002414 | Paxs    | 535.19 | Joback Method |
| dvisc | 0.0001847 | Paxs    | 581.99 | Joback Method |
| dvisc | 0.0001471 | Paxs    | 628.80 | Joback Method |

## Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 450.20 | K    | 2.70           | NIST Webbook |

## 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=C952807&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C952807&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>chs:</b>     | Standard solid enthalpy of combustion           |
| <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>hvac:</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>tbrp:</b> | Boiling point at reduced pressure |
| <b>tc:</b>   | Critical Temperature              |
| <b>tf:</b>   | Normal melting (fusion) point     |
| <b>vc:</b>   | Critical Volume                   |

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