

# Benzene, 1,1'-(1,2-ethanediyl)bis[4-methyl-

|                      |                                                                                                                                                                                                                                                                                    |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Bibenzyl, 4,4'-dimethyl-<br>«alpha»,«beta»-Di-p-tolylethane<br>p,p'-Dimethylbibenzyl<br>sym-Di-p-tolylethane<br>1,2-Di-p-tolylethane<br>4,4'-Dimethylbibenzyl<br>4,4'-Dimethyldibenzyl<br>1,2-di-para-Tolylethane<br>1,2-Di(p-methylphenyl)ethane<br>1,2-Bis(p-methylphenyl)ethane |
| Inchi:               | InChI=1S/C16H18/c1-13-3-7-15(8-4-13)11-12-16-9-5-14(2)6-10-16/h3-10H,11-12H2,1-2H3                                                                                                                                                                                                 |
| InchiKey:            | XCCQFUHBIRHLQT-UHFFFAOYSA-N                                                                                                                                                                                                                                                        |
| Formula:             | C16H18                                                                                                                                                                                                                                                                             |
| SMILES:              | Cc1ccc(CCc2ccc(C)cc2)cc1                                                                                                                                                                                                                                                           |
| Mol. weight [g/mol]: | 210.31                                                                                                                                                                                                                                                                             |
| CAS:                 | 538-39-6                                                                                                                                                                                                                                                                           |

## Physical Properties

| Property code | Value           | Unit    | Source         |
|---------------|-----------------|---------|----------------|
| chs           | -8826.50 ± 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            | 357.00 ± 4.00   | K       | NIST Webbook   |
| tf            | 355.00 ± 0.40   | K       | NIST Webbook   |
| tf            | 354.00 ± 3.00   | K       | NIST Webbook   |
| vc            | 0.716           | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 471.73    | J/mol×K | 628.80          | Joback Method |
| cpg           | 489.89    | J/mol×K | 667.45          | Joback Method |
| cpg           | 506.82    | J/mol×K | 706.11          | Joback Method |
| cpg           | 522.58    | J/mol×K | 744.76          | Joback Method |
| cpg           | 537.22    | J/mol×K | 783.42          | Joback Method |
| cpg           | 550.82    | J/mol×K | 822.07          | Joback Method |
| cpg           | 563.43    | J/mol×K | 860.73          | Joback Method |
| dvisc         | 0.0014473 | Pa×s    | 347.96          | Joback Method |
| dvisc         | 0.0007888 | Pa×s    | 394.77          | Joback Method |
| dvisc         | 0.0004889 | Pa×s    | 441.57          | Joback Method |
| dvisc         | 0.0003321 | Pa×s    | 488.38          | Joback Method |
| dvisc         | 0.0002414 | Pa×s    | 535.19          | Joback Method |
| dvisc         | 0.0001847 | Pa×s    | 581.99          | Joback Method |
| dvisc         | 0.0001471 | Pa×s    | 628.80          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 451.20 | K    | 2.40           | NIST Webbook |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C538396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C538396&amp;Units=SI</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>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>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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