

# Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-

Other names:

1,1'-(1,1,2,2-tetramethylethylene)dibenzene  
1,1'-[1,1,2,2-Tetramethyl-1,2-ethandiyl]bis[benzene]  
1,1,2,2-Tetramethyl-1,2-diphenylethane  
1,2-DIPHENYLTETRAMETHYLETHANE  
2,3-Dimethyl-2,3-diphenylbutane  
2,3-Diphenyl-2,3-dimethylbutane  
Bibenzyl, «alpha», «alpha», «alpha»', «alpha»'-tetramethyl-  
Bibenzyl, Â«alphaÂ», Â«alphaÂ», Â«alphaÂ»', Â«alphaÂ»'-tetramethyl-  
Bicumyl  
Butane, 2,3-dimethyl-2,3-diphenyl-  
DICUMENE  
Dicumyl  
Interox CC-DFB  
NSC 34859  
Perkadox 30  
«alpha», «alpha»'-Dicumyl  
Â«alphaÂ», Â«alphaÂ»'-Dicumyl

**Inchi:** InChI=1S/C18H22/c1-17(2,15-11-7-5-8-12-15)18(3,4)16-13-9-6-10-14-16/h5-14H,1-4H3

**InchiKey:** HGTUJZTUQFXBIH-UHFFFAOYSA-N

**Formula:** C18H22

**SMILES:** CC(C)(c1ccccc1)C(C)(C)c1ccccc1

**Mol. weight [g/mol]:** 238.37

**CAS:** 1889-67-4

## Physical Properties

| Property code | Value            | Unit   | Source         |
|---------------|------------------|--------|----------------|
| chs           | -10188.00 ± 3.00 | kJ/mol | NIST Webbook   |
| gf            | 331.18           | kJ/mol | Joback Method  |
| hf            | 57.00 ± 3.00     | kJ/mol | NIST Webbook   |
| hfs           | -39.30 ± 3.00    | kJ/mol | NIST Webbook   |
| hfus          | 15.63            | kJ/mol | Joback Method  |
| hsub          | 96.30            | kJ/mol | NIST Webbook   |
| hsub          | 96.70 ± 0.80     | kJ/mol | NIST Webbook   |
| hvap          | 57.62            | kJ/mol | Joback Method  |
| log10ws       | -4.91            |        | Crippen Method |
| logp          | 4.942            |        | Crippen Method |
| mcvol         | 216.960          | ml/mol | McGowan Method |

|    |               |                      |               |
|----|---------------|----------------------|---------------|
| pc | 1982.35       | kPa                  | Joback Method |
| tb | 658.14        | K                    | Joback Method |
| tc | 907.10        | K                    | Joback Method |
| tf | 392.00 ± 1.00 | K                    | NIST Webbook  |
| tf | 393.00 ± 4.00 | K                    | NIST Webbook  |
| vc | 0.805         | m <sup>3</sup> /kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value        | Unit    | Temperature [K] | Source        |
|---------------|--------------|---------|-----------------|---------------|
| cpg           | 686.23       | J/mol×K | 907.10          | Joback Method |
| cpg           | 672.45       | J/mol×K | 865.61          | Joback Method |
| cpg           | 657.54       | J/mol×K | 824.11          | Joback Method |
| cpg           | 641.33       | J/mol×K | 782.62          | Joback Method |
| cpg           | 623.65       | J/mol×K | 741.13          | Joback Method |
| cpg           | 604.33       | J/mol×K | 699.63          | Joback Method |
| cpg           | 583.19       | J/mol×K | 658.14          | Joback Method |
| cps           | 321.10       | J/mol×K | 298.00          | NIST Webbook  |
| dvisc         | 0.0005267    | Paxs    | 452.91          | Joback Method |
| dvisc         | 0.0000908    | Paxs    | 658.14          | Joback Method |
| dvisc         | 0.0027465    | Paxs    | 350.30          | Joback Method |
| dvisc         | 0.0001261    | Paxs    | 606.83          | Joback Method |
| dvisc         | 0.0001859    | Paxs    | 555.53          | Joback Method |
| dvisc         | 0.0002968    | Paxs    | 504.22          | Joback Method |
| dvisc         | 0.0010824    | Paxs    | 401.61          | Joback Method |
| hfust         | 25.52        | kJ/mol  | 392.00          | NIST Webbook  |
| hfust         | 25.52        | kJ/mol  | 392.00          | NIST Webbook  |
| hsubt         | 96.70 ± 0.80 | kJ/mol  | 320.50          | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.32072e+01                   |
| Coeff. B                    | -4.33074e+03                  |
| Coeff. C                    | -1.04892e+02                  |
| Temperature range (K), min. | 440.15                        |

|                             |        |
|-----------------------------|--------|
| Temperature range (K), max. | 653.15 |
|-----------------------------|--------|

| Information                 | Value  |
|-----------------------------|--|
| Property code               | pvap   |
| Equation                    | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A                    | 1.36853e+02  |
| Coeff. B                    | -1.44359e+04   |
| Coeff. C                    | -1.72116e+01   |
| Coeff. D                    | 5.92895e-06  |
| Temperature range (K), min. | 392.15   |
| Temperature range (K), max. | 805.00   |

## Sources

|   |   |
|---|---|
| <b>KDB Vapor Pressure Data:</b>             | <a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=811">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=811</a>                                       |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>   |
| <b>Crippen Method:</b>                      | <a href="https://www.chemed.com/doc/models/crippen_log10ws">https://www.chemed.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>   |
| <b>KDB:</b>                                 | <a href="https://www.thermo.com/files/research/kdb/mol/mol811.mol">https://www.thermo.com/files/research/kdb/mol/mol811.mol</a>   |
| <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=C1889674&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1889674&amp;Units=SI</a>   |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |

## Legend

|               |  |
|---------------|--|
| <b>chs:</b>   | Standard solid enthalpy of combustion                    |
| <b>cpg:</b>   | Ideal gas heat capacity                                  |
| <b>cps:</b>   | Solid phase 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>hfs:</b>   | Solid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions                |
| <b>hfust:</b> | Enthalpy of fusion at a given temperature                |
| <b>hsub:</b>  | Enthalpy of sublimation at standard conditions           |
| <b>hsubt:</b> | Enthalpy of sublimation at a given temperature           |
| <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>pvap:</b>    | Vapor 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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