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

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|---|---|
| **Other names:** | Benzene, 1,1'-(1,2-ethanediyl)bis*2-methyl- |
| **Inchi:** | 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 |
| **InchiKey:** | QFEPNMCDSBNJDB-UHFFFAOYSA-N |
| **Formula:** | C16H18 |
| **SMILES:** | Cc1ccccc1CCc1ccccc1C |
| **Mol. weight [g/mol]:** | 210.31 |
| **CAS:** | 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/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 |

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|---|---|---|---|---|
| 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 | 450.20 | K | 2.70 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C952807&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**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

**chs:** Standard solid enthalpy of combustion
**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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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