

Cyclobutane, 1,2-diphenyl, cis

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|-----------------------------|---|
| Inchi: | InChI=1S/C16H16/c1-3-7-13(8-4-1)15-11-12-16(15)14-9-5-2-6-10-14/h1-10,15-16H,11-1 |
| InchiKey: | AERGGMDNGDDGPI-IYBDPMFKSA-N |
| Formula: | C16H16 |
| SMILES: | c1ccc(C2CCC2c2ccccc2)cc1 |
| Mol. weight [g/mol]: | 208.30 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 349.60 | kJ/mol | Joback Method |
| hf | 145.79 | kJ/mol | Joback Method |
| hfus | 22.38 | kJ/mol | Joback Method |
| hvap | 55.54 | kJ/mol | Joback Method |
| log10ws | -4.55 | | Crippen Method |
| logp | 4.348 | | Crippen Method |
| mvol | 177.920 | ml/mol | McGowan Method |
| pc | 2576.72 | kPa | Joback Method |
| rinpol | 1640.00 | | NIST Webbook |
| rinpol | 1640.00 | | NIST Webbook |
| tb | 625.18 | K | Joback Method |
| tc | 881.09 | K | Joback Method |
| tf | 333.10 | K | Joback Method |
| vc | 0.663 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 461.63 | J/molxK | 625.18 | Joback Method |
| cpg | 550.39 | J/molxK | 838.44 | Joback Method |
| cpg | 535.66 | J/molxK | 795.79 | Joback Method |
| cpg | 519.54 | J/molxK | 753.14 | Joback Method |
| cpg | 501.91 | J/molxK | 710.48 | Joback Method |
| cpg | 482.65 | J/molxK | 667.83 | Joback Method |
| cpg | 563.88 | J/molxK | 881.09 | Joback Method |
| dvisc | 0.0003289 | Paxs | 625.18 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003938 | Paxs | 576.50 | Joback Method |
| dvisc | 0.0004875 | Paxs | 527.82 | Joback Method |
| dvisc | 0.0006302 | Paxs | 479.14 | Joback Method |
| dvisc | 0.0008633 | Paxs | 430.46 | Joback Method |
| dvisc | 0.0012816 | Paxs | 381.78 | Joback Method |
| dvisc | 0.0021353 | Paxs | 333.10 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R310046&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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

| | |
|-----------------|---|
| 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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/30-042-1/Cyclobutane-1-2-diphenyl-cis.pdf>

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