# 1,2,4,5-[2.2.2.2]Cyclophane

**Other names:** [2.2.2.2](1,2,4,5)Cyclophane
**Inchi:** InChI=1S/C20H20/c1-2-14-10-18-6-5-16-9-13(1)15-3-4-17(14)12-20(18)8-7-19(16)11-15/
**InchiKey:** VKBBYQHRVDUAIS-UHFFFAOYSA-N
**Formula:** C20H20
**SMILES:** c1c2c3cc4c1CCc1cc(c(cc1CC4)CC3)CC2
**Mol. weight [g/mol]:** 260.37
**CAS:** 54100-59-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 502.04 | kJ/mol | Joback Method |
| hf | 233.69 | kJ/mol | Joback Method |
| hfus | 26.60 | kJ/mol | Joback Method |
| hvap | 69.13 | kJ/mol | Joback Method |
| ie | 7.35 | eV | NIST Webbook |
| ie | 7.67 ± 0.02 | eV | NIST Webbook |
| log10ws | -5.88 | | Crippen Method |
| logp | 3.768 | | Crippen Method |
| mcvol | 212.560 | ml/mol | McGowan Method |
| pc | 2263.26 | kPa | Joback Method |
| tb | 770.20 | K | Joback Method |
| tc | 1024.71 | K | Joback Method |
| tf | 513.18 | K | Joback Method |
| vc | 0.822 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 625.77 | J/mol×K | 770.20 | Joback Method |
| cpg | 643.53 | J/mol×K | 812.62 | Joback Method |
| cpg | 660.28 | J/mol×K | 855.04 | Joback Method |
| cpg | 676.27 | J/mol×K | 897.45 | Joback Method |
| cpg | 691.75 | J/mol×K | 939.87 | Joback Method |
| cpg | 706.97 | J/mol×K | 982.29 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 722.18 | J/mol×K | 1024.71 | Joback Method |
| dvisc | 0.0033005 | Pa×s | 513.18 | Joback Method |
| dvisc | 0.0028682 | Pa×s | 556.02 | Joback Method |
| dvisc | 0.0025431 | Pa×s | 598.85 | Joback Method |
| dvisc | 0.0022914 | Pa×s | 641.69 | Joback Method |
| dvisc | 0.0020916 | Pa×s | 684.53 | Joback Method |
| dvisc | 0.0019300 | Pa×s | 727.36 | Joback Method |
| dvisc | 0.0017968 | Pa×s | 770.20 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C54100593&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

**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
**ie:** Ionization energy
**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
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

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