

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

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|-----------------------------|-----------------------------------------------------------------------------------|
| 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: | <chem>c1c2c3cc4c1CCc1cc(c(cc1CC4)CC3)CC2</chem> |
| 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/molxK | 770.20 | Joback Method |
| cpg | 643.53 | J/molxK | 812.62 | Joback Method |
| cpg | 660.28 | J/molxK | 855.04 | Joback Method |
| cpg | 676.27 | J/molxK | 897.45 | Joback Method |
| cpg | 691.75 | J/molxK | 939.87 | Joback Method |
| cpg | 706.97 | J/molxK | 982.29 | Joback Method |

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

Sources

| | |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C54100593&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 |

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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<https://www.chemeo.com/cid/15-465-9/1-2-4-5-2-2-2-2-Cyclophane.pdf>

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