# Cyclobenzaprine

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|---|---|
| **Other names:** | 1-Propanamine, 3-(5H-dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-<br>5H-Dibenzo(a,d)cycloheptene-«delta»5,«gamma»-propylamine, N,N-dimethyl-<br>N,N-Dimethyl-5H-dibenzo(a,d)cycloheptene-«delta»5,«gamma»-propylamine<br>5-(3-Dimetilaminopropiliden)-5H-dibenzo-(a,d)-ciclopentene<br>Proeptatriene<br>Proheptatriene<br>MK 130<br>Ro 4-1577<br>RP 9715<br>10,11-Dehydroamitriptyline<br>9715 R.P<br>Proheptatrien<br>3-(5H-Dibenzo[a,d]cyclohepten-5-ylidene)-N,N-dimethyl-1-propanamine |
| **Inchi:** | InChI=1S/C20H21N/c1-21(2)15-7-12-20-18-10-5-3-8-16(18)13-14-17-9-4-6-11-19(17)20/ |
| **InchiKey:** | JURKNVYFZMSNLP-UHFFFAOYSA-N |
| **Formula:** | C20H21N |
| **SMILES:** | CN(C)CCC=C1c2ccccc2C=Cc2ccccc21 |
| **Mol. weight [g/mol]:** | 275.39 |
| **CAS:** | 303-53-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 577.74 | kJ/mol | Joback Method |
| hf | 288.47 | kJ/mol | Joback Method |
| hfus | 36.49 | kJ/mol | Joback Method |
| hvap | 69.33 | kJ/mol | Joback Method |
| log10ws | -5.11 | | Crippen Method |
| logp | 4.554 | | Crippen Method |
| mcvol | 235.660 | ml/mol | McGowan Method |
| pc | 1923.67 | kPa | Joback Method |
| rinpol | 2248.00 | | NIST Webbook |
| rinpol | 2204.00 | | NIST Webbook |
| rinpol | 2248.00 | | NIST Webbook |
| tb | 749.97 | K | Joback Method |
| tc | 983.67 | K | Joback Method |
| tf | 458.81 | K | Joback Method |
| vc | 0.884 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 659.74 | J/mol×K | 749.97 | Joback Method |
| cpg | 677.08 | J/mol×K | 788.92 | Joback Method |
| cpg | 693.22 | J/mol×K | 827.87 | Joback Method |
| cpg | 708.31 | J/mol×K | 866.82 | Joback Method |
| cpg | 722.48 | J/mol×K | 905.77 | Joback Method |
| cpg | 735.88 | J/mol×K | 944.72 | Joback Method |
| cpg | 748.64 | J/mol×K | 983.67 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C303537&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **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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