# Prenylamine

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|---|---|
| **Other names:** | Benzenepropanamine, N-(1-methyl-2-phenylethyl)-«gamma»-phenyl-<br>Phenethylamine, N-(3,3-diphenylpropyl)-«alpha»-methyl-<br>B-436<br>Bismethin<br>Carditin<br>Corpax<br>N-(3,3-Diphenylpropyl)-«alpha»-methylphenaethylamin<br>N-(3,3-Diphenylpropyl)-«alpha»-methylphenethylamine<br>Elecor<br>Falliocor<br>Hostaginan<br>N-(1-Methyl-2-phenylethyl)-«gamma»-phenylbenzenepropanamine<br>1-Phenyl-2-(1',1'-diphenylpropyl-3'-amino)propane<br>N-(3'-Phenyl-2-propyl)-1,1-diphenyl-3-propyloamine<br>Segontin<br>Synadrin<br>Valecor<br>DL-Prenylamine<br>Prenylamine (vasodilator)<br>SAN 13-194<br>Sandoz 13-194 |
| **Inchi:** | InChI=1S/C24H27N/c1-20(19-21-11-5-2-6-12-21)25-18-17-24(22-13-7-3-8-14-22)23-15-9 |
| **InchiKey:** | IFFPICMESYHZPQ-UHFFFAOYSA-N |
| **Formula:** | C24H27N |
| **SMILES:** | CC(Cc1ccccc1)NCCC(c1ccccc1)c1ccccc1 |
| **Mol. weight [g/mol]:** | 329.48 |
| **CAS:** | 390-64-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 572.94 | kJ/mol | Joback Method |
| hf | 213.81 | kJ/mol | Joback Method |
| hfus | 38.09 | kJ/mol | Joback Method |
| hvap | 81.51 | kJ/mol | Joback Method |
| log10ws | -6.54 | | Crippen Method |
| logp | 5.429 | | Crippen Method |

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|---|---|---|---|
| mcvol | 287.720 | ml/mol | McGowan Method |
| pc | 1600.00 | kPa | Joback Method |
| rinpol | 2550.00 | | NIST Webbook |
| rinpol | 2557.00 | | NIST Webbook |
| rinpol | 2546.00 | | NIST Webbook |
| rinpol | 2540.00 | | NIST Webbook |
| tb | 877.85 | K | Joback Method |
| tc | 1120.94 | K | Joback Method |
| tf | 462.16 | K | Joback Method |
| vc | 1.079 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 890.61 | J/mol×K | 877.85 | Joback Method |
| cpg | 908.36 | J/mol×K | 918.37 | Joback Method |
| cpg | 924.67 | J/mol×K | 958.88 | Joback Method |
| cpg | 939.69 | J/mol×K | 999.40 | Joback Method |
| cpg | 953.56 | J/mol×K | 1039.91 | Joback Method |
| cpg | 966.43 | J/mol×K | 1080.43 | Joback Method |
| cpg | 978.43 | J/mol×K | 1120.94 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C390647&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

# 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

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|---|---|
| **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 |