# Verapamil

**Other names:** 5-((3,4-Dimethoxyphenethyl)methylamino)-2-(3,4-dimethoxyphenyl)-2-isopropylvaleronitri
Benzeneacetonitrile, «alpha»-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy-«alpha»-(1
Benzeneacetonitrile, Â«alphaÂ»-[3-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]propyl]-3,4-dimethoxy-Â«alpha
CP-16533-1
D-365
Dilacoran
Iproveratril
Valeronitrile, 5-((3,4-dimethoxyphenethyl)methylamino)-2-(3,4-dimethoxyphenyl)-2-isopropyl-
Vasolan
«alpha»-((N-Methyl-N-homoveratryl)-«gamma»-aminopropyl)-3,4-dimethoxyphenylaceton
Â«alphaÂ»-((N-Methyl-N-homoveratryl)-Â«gammaÂ»-aminopropyl)-3,4-dimethoxyphenyl

**Inchi:** InChI=1S/C27H38N2O4/c1-20(2)27(19-28,22-10-12-24(31-5)26(18-22)33-7)14-8-15-29(3
**InchiKey:** SGTNSNPWRIOYBX-UHFFFAOYSA-N
**Formula:** C27H38N2O4
**SMILES:** COc1ccc(CCN(C)CCCC(C#N)(c2ccc(OC)c(OC)c2)C(C)C)cc1OC
**Mol. weight [g/mol]:** 454.60
**CAS:** 52-53-9

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 187.12 | kJ/mol | Joback Method |
| hf | -483.93 | kJ/mol | Joback Method |
| hfus | 50.55 | kJ/mol | Joback Method |
| hvap | 103.37 | kJ/mol | Joback Method |
| log10ws | -4.15 | | Aqueous Solubility Prediction Method |
| logp | 5.093 | | Crippen Method |
| mcvol | 378.610 | ml/mol | McGowan Method |
| pc | 931.78 | kPa | Joback Method |
| rinpol | 3161.00 | | NIST Webbook |
| rinpol | 3150.00 | | NIST Webbook |
| rinpol | 3150.00 | | NIST Webbook |
| tb | 1090.97 | K | Joback Method |
| tc | 1335.66 | K | Joback Method |
| tf | 469.48 | K | Aqueous Solubility Prediction Method |
| vc | 1.431 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1288.74 | J/mol×K | 1090.97 | Joback Method |
| cpg | 1301.36 | J/mol×K | 1131.75 | Joback Method |
| cpg | 1312.12 | J/mol×K | 1172.53 | Joback Method |
| cpg | 1321.07 | J/mol×K | 1213.32 | Joback Method |
| cpg | 1328.27 | J/mol×K | 1254.10 | Joback Method |
| cpg | 1333.79 | J/mol×K | 1294.88 | Joback Method |
| cpg | 1337.68 | J/mol×K | 1335.66 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C52539&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method
**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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