# 2-Imidazoline, 2-benzhydroxymethyl

**Other names:** Diphenazoline
**Inchi:** InChI=1S/C17H18N2O/c1-3-7-14(8-4-1)17(15-9-5-2-6-10-15)20-13-16-18-11-12-19-16/h
**InchiKey:** RTZMBWHMKICABA-UHFFFAOYSA-N
**Formula:** C17H18N2O
**SMILES:** c1ccc(C(OCC2=NCCN2)c2ccccc2)cc1
**Mol. weight [g/mol]:** 266.34
**CAS:** 6703-39-5

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 478.72 | kJ/mol | Joback Method |
| hf | 177.26 | kJ/mol | Joback Method |
| hfus | 33.96 | kJ/mol | Joback Method |
| hvap | 74.50 | kJ/mol | Joback Method |
| log10ws | -3.54 | | Crippen Method |
| logp | 2.794 | | Crippen Method |
| mcvol | 213.540 | ml/mol | McGowan Method |
| pc | 2665.27 | kPa | Joback Method |
| rinpol | 2210.00 | | NIST Webbook |
| rinpol | 2275.00 | | NIST Webbook |
| rinpol | 2210.00 | | NIST Webbook |
| tb | 790.04 | K | Joback Method |
| tc | 1057.46 | K | Joback Method |
| tf | 546.41 | K | Joback Method |
| vc | 0.797 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 636.94 | J/mol×K | 790.04 | Joback Method |
| cpg | 655.07 | J/mol×K | 834.61 | Joback Method |
| cpg | 671.32 | J/mol×K | 879.18 | Joback Method |
| cpg | 685.77 | J/mol×K | 923.75 | Joback Method |
| cpg | 698.49 | J/mol×K | 968.32 | Joback Method |

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|---|---|---|---|---|
| cpg | 709.56 | J/mol×K | 1012.89 | Joback Method |
| cpg | 719.04 | J/mol×K | 1057.46 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6703395&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

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