# 1,2-Benzenediol, 4-(2-amino-1-hydroxypropyl)-

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|---|---|
| **Other names:** | Nordefrin |
| | Benzyl alcohol, «alpha»-(1-aminoethyl)-3,4-dihydroxy- |
| | «alpha»-(1-Aminoethyl)-3,4-dihydroxybenzyl alcohol |
| | 3,4-Dihydrophenyl-1-amino-2-propanol-1 |
| | (.+/-.)-3,4-Dihydroxynorephedrine |
| | Dihydroxyphenylpropanolamine |
| | Dioxynorepinephrine |
| | Isoadrenaline |
| | Methylnoradrenaline |
| | «alpha»-Methylnoradrenaline |
| | «alpha»-Methylnorepinephrine |
| | DL-«alpha»-Methylnorepinephrine |
| | l-«alpha»-Methylnorepinephrine |
| | Nordephrine |
| | 2-amino-1-(3,4-dihydroxyphenyl)propan-1-ol |
| **Inchi:** | InChI=1S/C9H13NO3/c1-5(10)9(13)6-2-3-7(11)8(12)4-6/h2-5,9,11-13H,10H2,1H3 |
| **InchiKey:** | GEFQWZLICWMTKF-UHFFFAOYSA-N |
| **Formula:** | C9H13NO3 |
| **SMILES:** | CC(N)C(O)c1ccc(O)c(O)c1 |
| **Mol. weight [g/mol]:** | 183.20 |
| **CAS:** | 6539-57-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -247.18 | kJ/mol | Joback Method |
| hf | -476.18 | kJ/mol | Joback Method |
| hfus | 26.91 | kJ/mol | Joback Method |
| hvap | 90.48 | kJ/mol | Joback Method |
| log10ws | -1.06 | | Crippen Method |
| logp | 0.478 | | Crippen Method |
| mcvol | 141.500 | ml/mol | McGowan Method |
| pc | 6027.93 | kPa | Joback Method |
| tb | 757.07 | K | Joback Method |
| tc | 986.21 | K | Joback Method |
| tf | 555.13 | K | Joback Method |
| vc | 0.400 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 409.54 | J/mol×K | 757.07 | Joback Method |
| cpg | 418.76 | J/mol×K | 795.26 | Joback Method |
| cpg | 427.63 | J/mol×K | 833.45 | Joback Method |
| cpg | 436.30 | J/mol×K | 871.64 | Joback Method |
| cpg | 444.89 | J/mol×K | 909.83 | Joback Method |
| cpg | 453.55 | J/mol×K | 948.02 | Joback Method |
| cpg | 462.41 | J/mol×K | 986.21 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6539577&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
**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume