# 4-Amino-1-butanol

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|---|---|
| **Other names:** | 4-hdyroxybutylamine |
| | H2NCH2(CH2)2CH2OH |
| | 4-Aminobutanol-1 |
| | 1-Butanol, 4-amino- |
| | 4-Aminobutanol |
| | NH2(CH2)4OH |
| **Inchi:** | InChI=1S/C4H11NO/c5-3-1-2-4-6/h6H,1-5H2 |
| **InchiKey:** | BLFRQYKZFKYQLO-UHFFFAOYSA-N |
| **Formula:** | C4H11NO |
| **SMILES:** | NCCCCO |
| **Mol. weight [g/mol]:** | 89.14 |
| **CAS:** | 13325-10-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 984.50 | kJ/mol | NIST Webbook |
| basg | 932.10 | kJ/mol | NIST Webbook |
| gf | -87.57 | kJ/mol | Joback Method |
| hf | -244.33 | kJ/mol | Joback Method |
| hfus | 15.40 | kJ/mol | Joback Method |
| hvap | 51.82 | kJ/mol | Joback Method |
| log10ws | -0.19 | | Crippen Method |
| logp | -0.282 | | Crippen Method |
| mcvol | 83.070 | ml/mol | McGowan Method |
| pc | 4736.62 | kPa | Joback Method |
| rinpol | 998.00 | | NIST Webbook |
| rinpol | 904.00 | | NIST Webbook |
| rinpol | 904.00 | | NIST Webbook |
| ripol | 1687.00 | | NIST Webbook |
| tb | 479.00 | K | NIST Webbook |
| tb | 476.00 ± 6.00 | K | NIST Webbook |
| tb | 479.20 | K | NIST Webbook |
| tc | 631.39 | K | Joback Method |
| tf | 278.92 | K | Joback Method |
| vc | 0.307 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 179.46 | J/mol×K | 455.63 | Joback Method |
| cpg | 187.25 | J/mol×K | 484.92 | Joback Method |
| cpg | 194.72 | J/mol×K | 514.22 | Joback Method |
| cpg | 201.89 | J/mol×K | 543.51 | Joback Method |
| cpg | 208.76 | J/mol×K | 572.80 | Joback Method |
| cpg | 215.33 | J/mol×K | 602.09 | Joback Method |
| cpg | 221.63 | J/mol×K | 631.39 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 398.20 | K | 4.50 | NIST Webbook |
| tbrp | 398.00 | K | 4.50 | NIST Webbook |

# Sources

**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=C13325105&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**affp:** Proton affinity
**basg:** Gas basicity
**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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |