# 1,3-Propanediamine, N,N'-bis(3-aminopropyl)-

| | |
|---|---|
| **Other names:** | N,N'-Bis(3-aminopropyl)-1,3-propanediamine |
| | 1,5,9,13-Tetraazatridecane |
| | N,N'-bis(3-aminopropyl)propane-1,3-diamine |
| **Inchi:** | InChI=1S/C9H24N4/c10-4-1-6-12-8-3-9-13-7-2-5-11/h12-13H,1-11H2 |
| **InchiKey:** | ZAXCZCOUDLENMH-UHFFFAOYSA-N |
| **Formula:** | C9H24N4 |
| **SMILES:** | NCCCNCCCNCCCN |
| **Mol. weight [g/mol]:** | 188.31 |
| **CAS:** | 4605-14-5 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 336.58 | kJ/mol | Joback Method |
| hf | -54.57 | kJ/mol | Joback Method |
| hfus | 39.66 | kJ/mol | Joback Method |
| hvap | 69.78 | kJ/mol | Joback Method |
| log10ws | -0.84 | | Crippen Method |
| logp | -0.747 | | Crippen Method |
| mcvol | 177.590 | ml/mol | McGowan Method |
| pc | 2651.56 | kPa | Joback Method |
| tb | 650.72 | K | Joback Method |
| tc | 839.79 | K | Joback Method |
| tf | 463.03 | K | Joback Method |
| vc | 0.667 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 506.96 | J/mol×K | 650.72 | Joback Method |
| cpg | 521.26 | J/mol×K | 682.23 | Joback Method |
| cpg | 534.84 | J/mol×K | 713.74 | Joback Method |
| cpg | 547.72 | J/mol×K | 745.25 | Joback Method |
| cpg | 559.93 | J/mol×K | 776.76 | Joback Method |
| cpg | 571.49 | J/mol×K | 808.28 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 582.42 | J/mol×K | 839.79 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 373.70 | K | 0.10 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C4605145&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
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point
**vc:** Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.