# Propanenitrile, 2,3-dibromo-

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|---|---|
| **Other names:** | 2,3-Dibromopropionitrile |
| | 1,2-Dibromopropionitrile |
| | 2,3-dibromopropiononitrile |
| **Inchi:** | InChI=1S/C3H3Br2N/c4-1-3(5)2-6/h3H,1H2 |
| **InchiKey:** | ARRIEYYNOLTVTE-UHFFFAOYSA-N |
| **Formula:** | C3H3Br2N |
| **SMILES:** | N#CC(Br)CBr |
| **Mol. weight [g/mol]:** | 212.87 |
| **CAS:** | 4554-16-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 133.76 | kJ/mol | Joback Method |
| hf | 107.01 | kJ/mol | Joback Method |
| hfus | 12.08 | kJ/mol | Joback Method |
| hvap | 45.23 | kJ/mol | Joback Method |
| log10ws | -1.92 | | Crippen Method |
| logp | 1.668 | | Crippen Method |
| mcvol | 89.510 | ml/mol | McGowan Method |
| pc | 5213.15 | kPa | Joback Method |
| tb | 446.20 | K | NIST Webbook |
| tc | 739.14 | K | Joback Method |
| tf | 293.16 | K | Joback Method |
| vc | 0.347 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 132.18 | J/mol×K | 502.00 | Joback Method |
| cpg | 136.55 | J/mol×K | 541.52 | Joback Method |
| cpg | 140.56 | J/mol×K | 581.05 | Joback Method |
| cpg | 144.25 | J/mol×K | 620.57 | Joback Method |
| cpg | 147.64 | J/mol×K | 660.10 | Joback Method |
| cpg | 150.77 | J/mol×K | 699.62 | Joback Method |

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|---|---|---|---|---|
| cpg | 153.67 | J/mol×K | 739.14 | Joback Method |

# 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=C4554169&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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