# Cyanogen bromide

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|---|---|
| **Other names:** | (CN)Br |
| | BrCN |
| | Bromine cyanide |
| | Bromine cyanide (BrCN) |
| | Bromine monocyanide |
| | Bromocyan |
| | Bromocyanide |
| | Bromocyanide (BrCN) |
| | Bromocyanogen |
| | Bromure de cyanogen |
| | Campilit |
| | Cyanobromide |
| | Cyanogen bromide ((CN)Br) |
| | Cyanogen bromide (BrCN) |
| | Cyanogen monobromide |
| | NSC 89684 |
| | Rcra waste number U246 |
| | TL 822 |
| | UN 1889 |
| **Inchi:** | InChI=1S/CBrN/c2-1-3 |
| **InchiKey:** | ATDGTVJJHBUTRL-UHFFFAOYSA-N |
| **Formula:** | CBrN |
| **SMILES:** | N#CBr |
| **Mol. weight [g/mol]:** | 105.92 |
| **CAS:** | 506-68-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 749.80 | kJ/mol | NIST Webbook |
| basg | 719.20 | kJ/mol | NIST Webbook |
| gf | 105.04 | kJ/mol | Joback Method |
| hf | 185.60 ± 6.00 | kJ/mol | NIST Webbook |
| hfs | 140.40 ± 4.30 | kJ/mol | NIST Webbook |
| hfus | 5.14 | kJ/mol | Joback Method |
| hsub | 45.23 | kJ/mol | NIST Webbook |
| hvap | 34.73 | kJ/mol | Joback Method |
| ie | 12.00 ± 1.00 | eV | NIST Webbook |

| | | | |
|---|---|---|---|
| ie | 11.88 | eV | NIST Webbook |
| ie | 11.84 ± 0.01 | eV | NIST Webbook |
| ie | 11.85 ± 0.02 | eV | NIST Webbook |
| log10ws | -1.03 | | Crippen Method |
| logp | 0.862 | | Crippen Method |
| mcvol | 43.830 | ml/mol | McGowan Method |
| pc | 6200.01 | kPa | Joback Method |
| rinpol | 482.00 | | NIST Webbook |
| rinpol | 482.00 | | NIST Webbook |
| tb | 390.52 | K | Joback Method |
| tc | 609.48 | K | Joback Method |
| tf | 225.82 | K | Joback Method |
| vc | 0.179 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 48.88 | J/mol×K | 500.00 | Joback Method |
| cpg | 49.66 | J/mol×K | 536.49 | Joback Method |
| cpg | 50.36 | J/mol×K | 572.99 | Joback Method |
| cpg | 46.08 | J/mol×K | 390.52 | Joback Method |
| cpg | 47.10 | J/mol×K | 427.01 | Joback Method |
| cpg | 48.03 | J/mol×K | 463.51 | Joback Method |
| cpg | 51.01 | J/mol×K | 609.48 | Joback Method |
| hsubt | 45.20 ± 4.20 | kJ/mol | 290.50 | NIST Webbook |
| hsubt | 45.90 | kJ/mol | 293.00 | NIST Webbook |
| hsubt | 47.00 | kJ/mol | 282.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.56682e+01 |
| Coeff. B | -2.78893e+03 |
| Coeff. C | -8.21550e+01 |
| Temperature range (K), min. | 260.15 |
| Temperature range (K), max. | 351.57 |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C506683&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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