# Butane, 2-bromo-2,3-dimethyl-

**Other names:** 2-Bromo-2,3-dimethylbutane
**Inchi:** InChI=1S/C6H13Br/c1-5(2)6(3,4)7/h5H,1-4H3
**InchiKey:** NILGDLGIGRGWRL-UHFFFAOYSA-N
**Formula:** C6H13Br
**SMILES:** CC(C)C(C)(C)Br
**Mol. weight [g/mol]:** 165.07
**CAS:** 594-52-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 14.36 | kJ/mol | Joback Method |
| hf | -154.87 | kJ/mol | Joback Method |
| hfus | 5.64 | kJ/mol | Joback Method |
| hvap | 33.70 | kJ/mol | Joback Method |
| log10ws | -2.64 | | Crippen Method |
| logp | 2.816 | | Crippen Method |
| mcvol | 112.900 | ml/mol | McGowan Method |
| pc | 3468.36 | kPa | Joback Method |
| rinpol | 903.00 | | NIST Webbook |
| rinpol | 921.00 | | NIST Webbook |
| rinpol | 896.00 | | NIST Webbook |
| rinpol | 903.00 | | NIST Webbook |
| ripol | 1035.00 | | NIST Webbook |
| ripol | 1035.00 | | NIST Webbook |
| ripol | 1028.00 | | NIST Webbook |
| ripol | 1053.00 | | NIST Webbook |
| tb | 399.17 | K | Joback Method |
| tc | 600.31 | K | Joback Method |
| tf | 204.60 | K | Joback Method |
| vc | 0.416 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 199.43 | J/mol×K | 399.17 | Joback Method |
| cpg | 211.94 | J/mol×K | 432.69 | Joback Method |
| cpg | 223.69 | J/mol×K | 466.22 | Joback Method |
| cpg | 234.74 | J/mol×K | 499.74 | Joback Method |
| cpg | 245.11 | J/mol×K | 533.26 | Joback Method |
| cpg | 254.84 | J/mol×K | 566.79 | Joback Method |
| cpg | 263.97 | J/mol×K | 600.31 | Joback Method |
| dvisc | 0.0112812 | Pa×s | 204.60 | Joback Method |
| dvisc | 0.0043112 | Pa×s | 237.03 | Joback Method |
| dvisc | 0.0020768 | Pa×s | 269.46 | Joback Method |
| dvisc | 0.0011704 | Pa×s | 301.88 | Joback Method |
| dvisc | 0.0007372 | Pa×s | 334.31 | Joback Method |
| dvisc | 0.0005039 | Pa×s | 366.74 | Joback Method |
| dvisc | 0.0003664 | Pa×s | 399.17 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.40255e+01 |
| Coeff. B | -3.44629e+03 |
| Coeff. C | -5.40600e+01 |
| Temperature range (K), min. | 298.15 |
| Temperature range (K), max. | 449.55 |

# 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=C594525&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

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |
| **pvap:** | Vapor pressure |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |