# 1,5-Dibromo-3-methylpentane

**Inchi:** InChI=1S/C6H12Br2/c1-6(2-4-7)3-5-8/h6H,2-5H2,1H3
**InchiKey:** YDPZWUMQKMLLHC-UHFFFAOYSA-N
**Formula:** C6H12Br2
**SMILES:** CC(CCBr)CCBr
**Mol. weight [g/mol]:** 243.97
**CAS:** 4457-72-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 25.84 | kJ/mol | Joback Method |
| hf | -119.79 | kJ/mol | Joback Method |
| hfus | 18.34 | kJ/mol | Joback Method |
| hvap | 41.43 | kJ/mol | Joback Method |
| log10ws | -2.96 | | Crippen Method |
| logp | 3.192 | | Crippen Method |
| mcvol | 130.400 | ml/mol | McGowan Method |
| pc | 3682.02 | kPa | Joback Method |
| tb | 468.56 | K | Joback Method |
| tc | 674.72 | K | Joback Method |
| tf | 261.98 | K | Joback Method |
| vc | 0.489 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 234.23 | J/mol×K | 468.56 | Joback Method |
| cpg | 244.92 | J/mol×K | 502.92 | Joback Method |
| cpg | 254.99 | J/mol×K | 537.28 | Joback Method |
| cpg | 264.50 | J/mol×K | 571.64 | Joback Method |
| cpg | 273.46 | J/mol×K | 606.00 | Joback Method |
| cpg | 281.92 | J/mol×K | 640.36 | Joback Method |
| cpg | 289.89 | J/mol×K | 674.72 | Joback Method |
| dvisc | 0.0043004 | Pa×s | 261.98 | Joback Method |
| dvisc | 0.0022284 | Pa×s | 296.41 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0013240 | Pa×s | 330.84 | Joback Method |
| dvisc | 0.0008678 | Pa×s | 365.27 | Joback Method |
| dvisc | 0.0006117 | Pa×s | 399.70 | Joback Method |
| dvisc | 0.0004558 | Pa×s | 434.13 | Joback Method |
| dvisc | 0.0003546 | Pa×s | 468.56 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.31886e+01 |
| Coeff. B | -3.70774e+03 |
| Coeff. C | -7.35200e+01 |
| Temperature range (K), min. | 360.92 |
| Temperature range (K), max. | 544.22 |

# 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=C4457721&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |