# Propane, 2-methyl-1,2,3-tribromo-

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|---|---|
| **Other names:** | 1,2,3-tribromo-2-methylpropane |
| **Inchi:** | InChI=1S/C4H7Br3/c1-4(7,2-5)3-6/h2-3H2,1H3 |
| **InchiKey:** | OIRQLILPXCJMIY-UHFFFAOYSA-N |
| **Formula:** | C4H7Br3 |
| **SMILES:** | CC(Br)(CBr)CBr |
| **Mol. weight [g/mol]:** | 294.81 |
| **CAS:** | 631-28-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 28.60 | kJ/mol | Joback Method |
| hf | -55.65 | kJ/mol | Joback Method |
| hfus | 14.56 | kJ/mol | Joback Method |
| hvap | 42.51 | kJ/mol | Joback Method |
| log10ws | -2.90 | | Crippen Method |
| logp | 2.930 | | Crippen Method |
| mcvol | 119.720 | ml/mol | McGowan Method |
| pc | 5281.57 | kPa | Joback Method |
| tb | 486.17 | K | Joback Method |
| tc | 726.33 | K | Joback Method |
| tf | 316.66 | K | Joback Method |
| vc | 0.434 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 189.99 | J/mol×K | 486.17 | Joback Method |
| cpg | 197.96 | J/mol×K | 526.20 | Joback Method |
| cpg | 205.14 | J/mol×K | 566.22 | Joback Method |
| cpg | 211.61 | J/mol×K | 606.25 | Joback Method |
| cpg | 217.45 | J/mol×K | 646.28 | Joback Method |
| cpg | 222.74 | J/mol×K | 686.30 | Joback Method |
| cpg | 227.56 | J/mol×K | 726.33 | Joback Method |
| dvisc | 0.0029905 | Pa×s | 316.66 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0018861 | Pa×s | 344.91 | Joback Method |
| dvisc | 0.0012755 | Pa×s | 373.16 | Joback Method |
| dvisc | 0.0009115 | Pa×s | 401.41 | Joback Method |
| dvisc | 0.0006807 | Pa×s | 429.67 | Joback Method |
| dvisc | 0.0005270 | Pa×s | 457.92 | Joback Method |
| dvisc | 0.0004204 | Pa×s | 486.17 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52873e+01 |
| Coeff. B | -4.40652e+03 |
| Coeff. C | -7.82460e+01 |
| Temperature range (K), min. | 372.02 |
| Temperature range (K), max. | 522.47 |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C631287&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 |

# 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 |

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|---|---|
| **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 |

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