# Acetaldehyde, tribromo-

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|---|---|
| **Other names:** | 2,2,2-Tribromoacetaldehyde |
| | Bromal |
| | Tribromoacetaldehyde |
| **Inchi:** | InChI=1S/C2HBr3O/c3-2(4,5)1-6/h1H |
| **InchiKey:** | YTGSYRVSBPFKMQ-UHFFFAOYSA-N |
| **Formula:** | C2HBr3O |
| **SMILES:** | O=CC(Br)(Br)Br |
| **Mol. weight [g/mol]:** | 280.74 |
| **CAS:** | 115-17-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -87.76 | kJ/mol | Joback Method |
| hf | -99.95 | kJ/mol | Joback Method |
| hfl | -88.70 | kJ/mol | NIST Webbook |
| hfus | 11.67 | kJ/mol | Joback Method |
| hvap | 44.77 | kJ/mol | Joback Method |
| log10ws | -2.34 | | Crippen Method |
| logp | 2.024 | | Crippen Method |
| mcvol | 93.110 | ml/mol | McGowan Method |
| pc | 8116.22 | kPa | Joback Method |
| tb | 447.20 | K | NIST Webbook |
| tb | 447.15 ± 1.50 | K | NIST Webbook |
| tc | 742.81 | K | Joback Method |
| tf | 336.12 | K | Joback Method |
| vc | 0.340 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 135.84 | J/mol×K | 742.81 | Joback Method |
| cpg | 123.08 | J/mol×K | 489.07 | Joback Method |
| cpg | 126.44 | J/mol×K | 531.36 | Joback Method |
| cpg | 129.20 | J/mol×K | 573.65 | Joback Method |

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|---|---|---|---|---|
| cpg | 131.43 | J/mol×K | 615.94 | Joback Method |
| cpg | 133.23 | J/mol×K | 658.23 | Joback Method |
| cpg | 134.67 | J/mol×K | 700.52 | Joback Method |
| dvisc | 0.0005919 | Pa×s | 489.07 | Joback Method |
| dvisc | 0.0031192 | Pa×s | 336.12 | Joback Method |
| dvisc | 0.0021446 | Pa×s | 361.61 | Joback Method |
| dvisc | 0.0015490 | Pa×s | 387.10 | Joback Method |
| dvisc | 0.0011648 | Pa×s | 412.60 | Joback Method |
| dvisc | 0.0009054 | Pa×s | 438.09 | Joback Method |
| dvisc | 0.0007235 | Pa×s | 463.58 | Joback Method |
| hvapt | 47.80 | kJ/mol | 369.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 334.20 | K | 1.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.60733e+01 |
| Coeff. B | -4.83596e+03 |
| Coeff. C | -2.49800e+01 |
| Temperature range (K), min. | 331.33 |
| Temperature range (K), max. | 474.34 |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C115173&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

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |