

Propane, 1,2,2-tribromo-

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|-----------------------------|--|
| Other names: | 1,2,2-Tribromopropane |
| Inchi: | InChI=1S/C3H5Br3/c1-3(5,6)2-4/h2H2,1H3 |
| InchiKey: | IELJYJRPJJILHQ-UHFFFAOYSA-N |
| Formula: | C3H5Br3 |
| SMILES: | CC(Br)(Br)CBr |
| Mol. weight [g/mol]: | 280.78 |
| CAS: | 14476-30-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 20.18 | kJ/mol | Joback Method |
| hf | -35.01 | kJ/mol | Joback Method |
| hfus | 11.97 | kJ/mol | Joback Method |
| hvap | 40.28 | kJ/mol | Joback Method |
| log10ws | -2.98 | | Crippen Method |
| logp | 2.887 | | Crippen Method |
| mcvol | 105.630 | ml/mol | McGowan Method |
| pc | 6103.52 | kPa | Joback Method |
| tb | 463.70 | K | NIST Webbook |
| tc | 707.88 | K | Joback Method |
| tf | 305.39 | K | Joback Method |
| vc | 0.379 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 152.43 | J/molxK | 463.29 | Joback Method |
| cpg | 158.97 | J/molxK | 504.05 | Joback Method |
| cpg | 164.77 | J/molxK | 544.82 | Joback Method |
| cpg | 169.90 | J/molxK | 585.58 | Joback Method |
| cpg | 174.44 | J/molxK | 626.35 | Joback Method |
| cpg | 178.48 | J/molxK | 667.11 | Joback Method |
| cpg | 182.09 | J/molxK | 707.88 | Joback Method |
| dvisc | 0.0031426 | Paxs | 305.39 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0020270 | Paxs | 331.71 | Joback Method |
| dvisc | 0.0013945 | Paxs | 358.02 | Joback Method |
| dvisc | 0.0010098 | Paxs | 384.34 | Joback Method |
| dvisc | 0.0007621 | Paxs | 410.66 | Joback Method |
| dvisc | 0.0005950 | Paxs | 436.97 | Joback Method |
| dvisc | 0.0004778 | Paxs | 463.29 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 354.20 | K | 2.70 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.51223e+01 |
| Coeff. B | -4.13350e+03 |
| Coeff. C | -7.01840e+01 |
| Temperature range (K), min. | 348.82 |
| Temperature range (K), max. | 492.10 |

Sources

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|---|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C14476303&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/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| h vap: | 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 |
| p vap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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