# Pentane, 1,2-dibromo-

**Other names:** Pentane, 1,2-dibromo-
**Inchi:** InChI=1S/C5H10Br2/c1-2-3-5(7)4-6/h5H,2-4H2,1H3
**InchiKey:** CITMYAPULDSOHG-UHFFFAOYSA-N
**Formula:** C5H10Br2
**SMILES:** CCCC(Br)CBr
**Mol. weight [g/mol]:** 229.94

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -114.74 | kJ/mol | Cheméo Relay (1.0) |
| hfl | -164.80 | kJ/mol | NIST Webbook |
| hfus | 15.75 | kJ/mol | Joback Method |
| hvap | 49.00 | kJ/mol | NIST Webbook |
| hvap | 49.20 ± 0.80 | kJ/mol | NIST Webbook |
| log10ws | -3.23 | | Cheméo Relay (1.0) |
| logp | 2.945 | | Crippen Method |
| mcvol | 116.310 | ml/mol | McGowan Method |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1056.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| rinpol | 1056.00 | | NIST Webbook |
| rinpol | 1033.00 | | NIST Webbook |
| tb | 438.89 | K | Cheméo Relay (1.0) |
| tf | 218.04 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 243.97 | J/mol×K | 654.58 | Joback Method |
| cpg | 229.60 | J/mol×K | 584.95 | Joback Method |
| cpg | 195.09 | J/mol×K | 445.68 | Joback Method |
| cpg | 204.52 | J/mol×K | 480.50 | Joback Method |
| cpg | 213.39 | J/mol×K | 515.31 | Joback Method |
| cpg | 221.74 | J/mol×K | 550.13 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 237.00 | J/mol×K | 619.76 | Joback Method |
| dvisc | 0.0043813 | Pa×s | 250.71 | Joback Method |
| dvisc | 0.0023206 | Pa×s | 283.20 | Joback Method |
| dvisc | 0.0014009 | Pa×s | 315.70 | Joback Method |
| dvisc | 0.0009293 | Pa×s | 348.19 | Joback Method |
| dvisc | 0.0006612 | Pa×s | 380.69 | Joback Method |
| dvisc | 0.0004963 | Pa×s | 413.19 | Joback Method |
| dvisc | 0.0003884 | Pa×s | 445.68 | Joback Method |
| hvapt | 46.50 | kJ/mol | 406.50 | NIST Webbook |
| hvapt | 48.80 | kJ/mol | 370.00 | NIST Webbook |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3234499&Units=SI
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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
**rinpol:** Non-polar retention indices
**tb:** Normal Boiling Point Temperature
**tf:** Normal melting (fusion) point

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