# trans-1,2-Dibromocycloheptane

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|---|---|
| **Inchi:** | InChI=1S/C7H12Br2/c8-6-4-2-1-3-5-7(6)9/h6-7H,1-5H2/t6-,7+ |
| **InchiKey:** | PQKOJNVKGNOTKZ-KNVOCYPGSA-N |
| **Formula:** | C7H12Br2 |
| **SMILES:** | BrC1CCCCCC1Br |
| **Mol. weight [g/mol]:** | 255.98 |
| **CAS:** | 52021-35-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 41.34 | kJ/mol | Joback Method |
| hf | -107.33 | kJ/mol | Joback Method |
| hfus | 15.26 | kJ/mol | Joback Method |
| hvap | 52.02 | kJ/mol | NIST Webbook |
| log10ws | -3.73 | | Crippen Method |
| logp | 3.478 | | Crippen Method |
| mcvol | 133.630 | ml/mol | McGowan Method |
| pc | 4135.61 | kPa | Joback Method |
| tb | 511.03 | K | Joback Method |
| tc | 761.30 | K | Joback Method |
| tf | 287.87 | K | Joback Method |
| vc | 0.475 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 260.05 | J/mol×K | 511.03 | Joback Method |
| cpg | 276.72 | J/mol×K | 552.74 | Joback Method |
| cpg | 292.25 | J/mol×K | 594.45 | Joback Method |
| cpg | 306.68 | J/mol×K | 636.16 | Joback Method |
| cpg | 320.06 | J/mol×K | 677.87 | Joback Method |
| cpg | 332.42 | J/mol×K | 719.58 | Joback Method |
| cpg | 343.80 | J/mol×K | 761.30 | Joback Method |
| dvisc | 0.0038417 | Pa×s | 287.87 | Joback Method |
| dvisc | 0.0020105 | Pa×s | 325.06 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0012019 | Pa×s | 362.26 | Joback Method |
| dvisc | 0.0007907 | Pa×s | 399.45 | Joback Method |
| dvisc | 0.0005586 | Pa×s | 436.64 | Joback Method |
| dvisc | 0.0004168 | Pa×s | 473.84 | Joback Method |
| dvisc | 0.0003245 | Pa×s | 511.03 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C52021359&Units=SI |
| **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 |

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

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