# 1-Bromo-5-methylhexane

**Inchi:** InChI=1S/C7H15Br/c1-7(2)5-3-4-6-8/h7H,3-6H2,1-2H3
**InchiKey:** XAOFMTDKQYEOES-UHFFFAOYSA-N
**Formula:** C7H15Br
**SMILES:** CC(C)CCCCBr
**Mol. weight [g/mol]:** 179.10
**CAS:** 35354-37-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 19.94 | kJ/mol | Joback Method |
| hf | -166.76 | kJ/mol | Joback Method |
| hfus | 15.65 | kJ/mol | Joback Method |
| hvap | 37.22 | kJ/mol | Joback Method |
| log10ws | -2.94 | | Crippen Method |
| logp | 3.208 | | Crippen Method |
| mcvol | 126.990 | ml/mol | McGowan Method |
| pc | 3042.32 | kPa | Joback Method |
| tb | 425.28 | K | Joback Method |
| tc | 611.91 | K | Joback Method |
| tf | 213.45 | K | Joback Method |
| vc | 0.483 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 236.30 | J/mol×K | 425.28 | Joback Method |
| cpg | 248.56 | J/mol×K | 456.38 | Joback Method |
| cpg | 260.26 | J/mol×K | 487.49 | Joback Method |
| cpg | 271.43 | J/mol×K | 518.59 | Joback Method |
| cpg | 282.08 | J/mol×K | 549.70 | Joback Method |
| cpg | 292.23 | J/mol×K | 580.80 | Joback Method |
| cpg | 301.90 | J/mol×K | 611.91 | Joback Method |
| dvisc | 0.0064391 | Pa×s | 213.45 | Joback Method |
| dvisc | 0.0027270 | Pa×s | 248.75 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0014299 | Pa×s | 284.06 | Joback Method |
| dvisc | 0.0008648 | Pa×s | 319.37 | Joback Method |
| dvisc | 0.0005781 | Pa×s | 354.67 | Joback Method |
| dvisc | 0.0004157 | Pa×s | 389.98 | Joback Method |
| dvisc | 0.0003157 | Pa×s | 425.28 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52627e+01 |
| Coeff. B | -4.03730e+03 |
| Coeff. C | -6.40400e+01 |
| Temperature range (K), min. | 333.64 |
| Temperature range (K), max. | 469.75 |

# Sources

**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=C35354371&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

**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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