# Octane, 2-bromo-

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|---|---|
| **Other names:** | (dl) 2-bromooctane |
| | 1-Methylheptyl bromide |
| | 2-Bromooctane |
| | 2-Bromoooctane |
| | 2-Octyl bromide |
| | sec-Octyl Bromide |
| **Inchi:** | InChI=1S/C8H17Br/c1-3-4-5-6-7-8(2)9/h8H,3-7H2,1-2H3 |
| **InchiKey:** | FTJHYGJLHCGQHQ-UHFFFAOYSA-N |
| **Formula:** | C8H17Br |
| **SMILES:** | CCCCCCC(C)Br |
| **Mol. weight [g/mol]:** | 193.12 |
| **CAS:** | 557-35-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 28.36 | kJ/mol | Joback Method |
| hf | -187.40 | kJ/mol | Joback Method |
| hfus | 18.24 | kJ/mol | Joback Method |
| hvap | 39.45 | kJ/mol | Joback Method |
| log10ws | -3.71 | | Crippen Method |
| logp | 3.740 | | Crippen Method |
| mcvol | 141.080 | ml/mol | McGowan Method |
| pc | 2744.03 | kPa | Joback Method |
| rinpol | 1093.00 | | NIST Webbook |
| rinpol | 1093.00 | | NIST Webbook |
| tb | 448.16 | K | Joback Method |
| tc | 633.14 | K | Joback Method |
| tf | 224.72 | K | Joback Method |
| vc | 0.539 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 348.69 | J/mol×K | 633.14 | Joback Method |

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|---|---|---|---|---|
| cpg | 277.18 | J/mol×K | 448.16 | Joback Method |
| cpg | 290.54 | J/mol×K | 478.99 | Joback Method |
| cpg | 303.29 | J/mol×K | 509.82 | Joback Method |
| cpg | 315.46 | J/mol×K | 540.65 | Joback Method |
| cpg | 327.07 | J/mol×K | 571.48 | Joback Method |
| cpg | 338.14 | J/mol×K | 602.31 | Joback Method |
| dvisc | 0.0002948 | Pa×s | 448.16 | Joback Method |
| dvisc | 0.0063866 | Pa×s | 224.72 | Joback Method |
| dvisc | 0.0026570 | Pa×s | 261.96 | Joback Method |
| dvisc | 0.0013751 | Pa×s | 299.20 | Joback Method |
| dvisc | 0.0008234 | Pa×s | 336.44 | Joback Method |
| dvisc | 0.0005461 | Pa×s | 373.68 | Joback Method |
| dvisc | 0.0003902 | Pa×s | 410.92 | Joback Method |
| hvapt | 48.40 | kJ/mol | 403.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.50922e+01 |
| Coeff. B | -4.14278e+03 |
| Coeff. C | -6.94890e+01 |
| Temperature range (K), min. | 349.32 |
| Temperature range (K), max. | 493.06 |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C557357&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

# 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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |