# Butane, 2-iodo-

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|---|---|
| **Other names:** | 2-Butyl Iodide |
| | 2-IODOBUTANE |
| | 2-Jodbutan |
| | SEC-BUTYL IODIDE |
| | SEC-IODOBUTANE |
| | UN 2390 |
| | sec-C4H9I |
| **Inchi:** | InChI=1S/C4H9I/c1-3-4(2)5/h4H,3H2,1-2H3 |
| **InchiKey:** | IQRUSQUYPCHEKN-UHFFFAOYSA-N |
| **Formula:** | C4H9I |
| **SMILES:** | CCC(C)I |
| **Mol. weight [g/mol]:** | 184.02 |
| **CAS:** | 513-48-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 38.48 | kJ/mol | Joback Method |
| hf | -54.30 | kJ/mol | Joback Method |
| hfus | 7.00 | kJ/mol | Joback Method |
| hvap | 37.90 | kJ/mol | NIST Webbook |
| hvap | 38.49 | kJ/mol | NIST Webbook |
| hvap | 38.46 ± 0.06 | kJ/mol | NIST Webbook |
| hvap | 38.50 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 38.80 | kJ/mol | NIST Webbook |
| ie | 9.40 | eV | NIST Webbook |
| ie | 9.09 ± 0.02 | eV | NIST Webbook |
| ie | 9.13 | eV | NIST Webbook |
| ie | 9.10 | eV | NIST Webbook |
| ie | 9.10 | eV | NIST Webbook |
| ie | 9.10 ± 0.02 | eV | NIST Webbook |
| log10ws | -2.56 | | Crippen Method |
| logp | 2.220 | | Crippen Method |
| mcvol | 93.040 | ml/mol | McGowan Method |
| pc | 3829.28 | kPa | Joback Method |
| rinpol | 789.00 | | NIST Webbook |
| ripol | 1019.00 | | NIST Webbook |
| ripol | 1019.00 | | NIST Webbook |

| | | | |
|---|---|---|---|
| tb | 392.70 ± 2.00 | K | NIST Webbook |
| tb | 393.00 | K | NIST Webbook |
| tb | 393.20 | K | NIST Webbook |
| tb | 392.70 | K | NIST Webbook |
| tb | 391.40 ± 1.00 | K | NIST Webbook |
| tb | 391.15 ± 1.50 | K | NIST Webbook |
| tb | 393.15 | K | KDB |
| tc | 593.02 | K | Joback Method |
| tf | 168.95 ± 0.40 | K | NIST Webbook |
| tf | 133.15 | K | KDB |
| vc | 0.342 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 137.04 | J/mol×K | 383.62 | Joback Method |
| cpg | 145.49 | J/mol×K | 418.52 | Joback Method |
| cpg | 153.49 | J/mol×K | 453.42 | Joback Method |
| cpg | 161.06 | J/mol×K | 488.32 | Joback Method |
| cpg | 168.23 | J/mol×K | 523.22 | Joback Method |
| cpg | 175.01 | J/mol×K | 558.12 | Joback Method |
| cpg | 181.41 | J/mol×K | 593.02 | Joback Method |
| cpl | 165.30 | J/mol×K | 298.15 | NIST Webbook |
| dvisc | 0.0101698 | Pa×s | 177.90 | Joback Method |
| dvisc | 0.0038120 | Pa×s | 212.19 | Joback Method |
| dvisc | 0.0018774 | Pa×s | 246.47 | Joback Method |
| dvisc | 0.0010993 | Pa×s | 280.76 | Joback Method |
| dvisc | 0.0007232 | Pa×s | 315.05 | Joback Method |
| dvisc | 0.0005165 | Pa×s | 349.33 | Joback Method |
| dvisc | 0.0003918 | Pa×s | 383.62 | Joback Method |
| hvapt | 33.27 | kJ/mol | 393.20 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.76031e+01 |

| | |
|---|---|
| Coeff. B | -5.19995e+03 |
| Coeff. C | 8.46400e+00 |
| Temperature range (K), min. | 291.84 |
| Temperature range (K), max. | 414.58 |

# Sources

| | |
|---|---|
| **KDB:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1612 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C513484&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 |
| **cpl:** | Liquid phase 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 |
| **ie:** | Ionization energy |
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |