# 3,4-Hexanedione

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|---|---|
| **Other names:** | 3,4-Hexandione |
| | Bipropionyl |
| | hexane-3,4-dione |
| **Inchi:** | InChI=1S/C6H10O2/c1-3-5(7)6(8)4-2/h3-4H2,1-2H3 |
| **InchiKey:** | KVFQMAZOBTXCAZ-UHFFFAOYSA-N |
| **Formula:** | C6H10O2 |
| **SMILES:** | CCC(=O)C(=O)CC |
| **Mol. weight [g/mol]:** | 114.14 |
| **CAS:** | 4437-51-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -258.20 | kJ/mol | Joback Method |
| hf | -392.33 | kJ/mol | Joback Method |
| hfus | 14.49 | kJ/mol | Joback Method |
| hvap | 42.44 | kJ/mol | Joback Method |
| log10ws | -0.89 | | Crippen Method |
| logp | 0.945 | | Crippen Method |
| mcvol | 98.540 | ml/mol | McGowan Method |
| pc | 3594.25 | kPa | Joback Method |
| rinpol | 801.00 | | NIST Webbook |
| rinpol | 804.00 | | NIST Webbook |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 816.00 | | NIST Webbook |
| rinpol | 773.40 | | NIST Webbook |
| rinpol | 773.00 | | NIST Webbook |
| rinpol | 777.00 | | NIST Webbook |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 800.00 | | NIST Webbook |
| rinpol | 804.00 | | NIST Webbook |
| rinpol | 801.00 | | NIST Webbook |
| rinpol | 777.00 | | NIST Webbook |
| ripol | 1157.00 | | NIST Webbook |
| ripol | 1135.00 | | NIST Webbook |
| ripol | 1151.00 | | NIST Webbook |
| ripol | 1123.00 | | NIST Webbook |
| ripol | 1140.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1183.00 | | NIST Webbook |
| ripol | 1143.00 | | NIST Webbook |
| ripol | 1143.00 | | NIST Webbook |
| ripol | 1143.00 | | NIST Webbook |
| ripol | 1164.00 | | NIST Webbook |
| ripol | 1151.00 | | NIST Webbook |
| ripol | 1164.00 | | NIST Webbook |
| ripol | 1135.00 | | NIST Webbook |
| tb | 397.20 | K | NIST Webbook |
| tb | 403.20 | K | NIST Webbook |
| tc | 634.10 | K | Joback Method |
| tf | 257.24 | K | Joback Method |
| vc | 0.384 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 193.61 | J/mol×K | 444.42 | Joback Method |
| cpg | 237.09 | J/mol×K | 602.49 | Joback Method |
| cpg | 229.18 | J/mol×K | 570.87 | Joback Method |
| cpg | 220.89 | J/mol×K | 539.26 | Joback Method |
| cpg | 212.20 | J/mol×K | 507.65 | Joback Method |
| cpg | 203.11 | J/mol×K | 476.03 | Joback Method |
| cpg | 244.62 | J/mol×K | 634.10 | Joback Method |
| dvisc | 0.0003624 | Pa×s | 444.42 | Joback Method |
| dvisc | 0.0004571 | Pa×s | 413.22 | Joback Method |
| dvisc | 0.0005990 | Pa×s | 382.03 | Joback Method |
| dvisc | 0.0008236 | Pa×s | 350.83 | Joback Method |
| dvisc | 0.0012049 | Pa×s | 319.63 | Joback Method |
| dvisc | 0.0019141 | Pa×s | 288.44 | Joback Method |
| dvisc | 0.0034020 | Pa×s | 257.24 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.55380e+01 |

| | |
|---|---|
| Coeff. B | -3.75609e+03 |
| Coeff. C | -5.32260e+01 |
| Temperature range (K), min. | 299.52 |
| Temperature range (K), max. | 420.51 |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4437518&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |

# 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 |
| **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 |

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