# Isocrotonic acid

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|---|---|
| **Other names:** | (2Z)-2-Butenoic acid |
| | (Z)-2-BUTENOIC ACID |
| | (Z)-CH3CH=CHCOOH |
| | (Z)-CROTONIC ACID |
| | 2-Butenoic acid, (Z)- |
| | CIS-CROTONIC ACID |
| | Crotonic acid, (Z)- |
| | cis-2-Butenoic Acid |
| **Inchi:** | InChI=1S/C4H6O2/c1-2-3-4(5)6/h2-3H,1H3,(H,5,6)/b3-2- |
| **InchiKey:** | LDHQCZJRKDOVOX-IHWYPQMZSA-N |
| **Formula:** | C4H6O2 |
| **SMILES:** | CC=CC(=O)O |
| **Mol. weight [g/mol]:** | 86.09 |
| **CAS:** | 503-64-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -202.72 | kJ/mol | Joback Method |
| hf | -273.48 | kJ/mol | Joback Method |
| hfus | 12.01 | kJ/mol | Joback Method |
| hvap | 47.88 | kJ/mol | Joback Method |
| ie | 10.08 | eV | NIST Webbook |
| log10ws | -0.45 | | Crippen Method |
| logp | 0.647 | | Crippen Method |
| mcvol | 70.360 | ml/mol | McGowan Method |
| pc | 4703.44 ± 100.00 | kPa | NIST Webbook |
| tb | 442.50 | K | NIST Webbook |
| tc | 644.60 ± 3.00 | K | NIST Webbook |
| tf | 240.51 | K | Joback Method |
| vc | 0.265 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

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|---|---|---|---|---|
| cpg | 161.26 | J/mol×K | 623.44 | Joback Method |
| cpg | 129.47 | J/mol×K | 441.13 | Joback Method |
| cpg | 135.50 | J/mol×K | 471.51 | Joback Method |
| cpg | 141.22 | J/mol×K | 501.90 | Joback Method |
| cpg | 146.65 | J/mol×K | 532.28 | Joback Method |
| cpg | 151.79 | J/mol×K | 562.67 | Joback Method |
| cpg | 156.65 | J/mol×K | 593.05 | Joback Method |
| dvisc | 0.0002256 | Pa×s | 441.13 | Joback Method |
| dvisc | 0.0325411 | Pa×s | 240.51 | Joback Method |
| dvisc | 0.0085700 | Pa×s | 273.95 | Joback Method |
| dvisc | 0.0030171 | Pa×s | 307.38 | Joback Method |
| dvisc | 0.0013037 | Pa×s | 340.82 | Joback Method |
| dvisc | 0.0006544 | Pa×s | 374.26 | Joback Method |
| dvisc | 0.0003678 | Pa×s | 407.69 | Joback Method |
| hfust | 12.57 | kJ/mol | 344.40 | NIST Webbook |
| hfust | 12.57 | kJ/mol | 344.40 | NIST Webbook |
| hvapt | 55.80 | kJ/mol | 375.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.57701e+01 |
| Coeff. B | -4.10684e+03 |
| Coeff. C | -7.42330e+01 |
| Temperature range (K), min. | 339.49 |
| Temperature range (K), max. | 470.28 |

# Sources

**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

**KDB:** https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=974

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

# 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |