# 2-Hexenoic acid, (E)-

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|---|---|
| **Other names:** | (2E)-2-Hexenoic acid |
| | (2E)-Hexenoic acid |
| | (E)-2-Hexenoic acid |
| | 2-Hexenoic acid, trans- |
| | trans-2-Hexenoic acid |
| | trans-hex-2-enoic acid |
| **Inchi:** | InChI=1S/C6H10O2/c1-2-3-4-5-6(7)8/h4-5H,2-3H2,1H3,(H,7,8)/b5-4+ |
| **InchiKey:** | NIONDZDPPYHYKY-SNAWJCMRSA-N |
| **Formula:** | C6H10O2 |
| **SMILES:** | CCCC=CC(=O)O |
| **Mol. weight [g/mol]:** | 114.14 |
| **CAS:** | 13419-69-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -185.88 | kJ/mol | Joback Method |
| hf | -314.76 | kJ/mol | Joback Method |
| hfus | 17.19 | kJ/mol | Joback Method |
| hvap | 52.33 | kJ/mol | Joback Method |
| log10ws | -1.29 | | Crippen Method |
| logp | 1.427 | | Crippen Method |
| mcvol | 98.540 | ml/mol | McGowan Method |
| pc | 3970.51 | kPa | Joback Method |
| rinpol | 1042.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| rinpol | 1042.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| ripol | 1951.00 | | NIST Webbook |
| ripol | 1951.00 | | NIST Webbook |
| ripol | 1933.00 | | NIST Webbook |
| ripol | 1941.00 | | NIST Webbook |
| ripol | 1967.00 | | NIST Webbook |
| ripol | 1922.00 | | NIST Webbook |
| ripol | 1967.00 | | NIST Webbook |
| ripol | 1967.00 | | NIST Webbook |
| ripol | 1938.00 | | NIST Webbook |
| ripol | 2002.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1967.00 | | NIST Webbook |
| ripol | 1962.00 | | NIST Webbook |
| ripol | 1970.00 | | NIST Webbook |
| ripol | 1969.00 | | NIST Webbook |
| ripol | 1971.00 | | NIST Webbook |
| ripol | 1922.00 | | NIST Webbook |
| ripol | 1983.00 | | NIST Webbook |
| tb | 490.20 | K | NIST Webbook |
| tc | 665.94 | K | Joback Method |
| tf | 307.65 ± 1.00 | K | NIST Webbook |
| vc | 0.377 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 206.08 | J/mol×K | 486.89 | Joback Method |
| cpg | 214.50 | J/mol×K | 516.73 | Joback Method |
| cpg | 222.51 | J/mol×K | 546.57 | Joback Method |
| cpg | 230.13 | J/mol×K | 576.41 | Joback Method |
| cpg | 237.37 | J/mol×K | 606.26 | Joback Method |
| cpg | 244.26 | J/mol×K | 636.10 | Joback Method |
| cpg | 250.80 | J/mol×K | 665.94 | Joback Method |
| dvisc | 0.0232383 | Pa×s | 263.05 | Joback Method |
| dvisc | 0.0061439 | Pa×s | 300.36 | Joback Method |
| dvisc | 0.0021795 | Pa×s | 337.66 | Joback Method |
| dvisc | 0.0009502 | Pa×s | 374.97 | Joback Method |
| dvisc | 0.0004814 | Pa×s | 412.28 | Joback Method |
| dvisc | 0.0002731 | Pa×s | 449.58 | Joback Method |
| dvisc | 0.0001689 | Pa×s | 486.89 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.56880e+01 |
| Coeff. B | -4.56942e+03 |
| Coeff. C | -7.74120e+01 |

| | |
|---|---|
| Temperature range (K), min. | 374.12 |
| Temperature range (K), max. | 517.77 |

# 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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13419697&Units=SI |

# 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 |