# 1,11-Undecanedioic acid

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|---|---|
| **Other names:** | .alpha.,.omega.-tridecanedioic acid |
| | 1,11-undecanedicarboxylic acid |
| | 1,13-tridecanedioic acid |
| | Brassilic acid |
| | brassylic acid |
| | tridecanedioic acid |
| **Inchi:** | InChI=1S/C13H24O4/c14-12(15)10-8-6-4-2-1-3-5-7-9-11-13(16)17/h1-11H2,(H,14,15)(H, |
| **InchiKey:** | DXNCZXXFRKPEPY-UHFFFAOYSA-N |
| **Formula:** | C13H24O4 |
| **SMILES:** | O=C(O)CCCCCCCCCCCC(=O)O |
| **Mol. weight [g/mol]:** | 244.33 |
| **CAS:** | 505-52-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 1.1048 | | Cheméo Relay (1.0) |
| chs | -7397.30 ± 3.30 | kJ/mol | NIST Webbook |
| gf | -472.90 | kJ/mol | Joback Method |
| hf | -984.11 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 49.40 | kJ/mol | Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16 |
| hvap | 137.74 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.76 | eV | Cheméo Relay (1.0) |
| log10ws | -3.55 | | Cheméo Relay (1.0) |
| logp | 3.447 | | Crippen Method |
| mcvol | 208.910 | ml/mol | McGowan Method |
| pc | 2151.31 | kPa | Joback Method |
| tb | 580.31 | K | Cheméo Relay (1.0) |
| tc | 801.56 | K | Cheméo Relay (1.0) |
| tf | 387.50 ± 0.50 | K | NIST Webbook |
| tf | 386.21 | K | Solubility of tridecanedioic acid in pure solvent systems: An experimental and computational study |
| vc | 0.797 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 696.66 | J/mol×K | 968.90 | Joback Method |
| cpg | 634.46 | J/mol×K | 788.94 | Joback Method |
| cpg | 646.32 | J/mol×K | 818.93 | Joback Method |
| cpg | 657.56 | J/mol×K | 848.93 | Joback Method |
| cpg | 668.18 | J/mol×K | 878.92 | Joback Method |
| cpg | 678.23 | J/mol×K | 908.91 | Joback Method |
| cpg | 687.71 | J/mol×K | 938.90 | Joback Method |
| dvisc | 0.0011525 | Pa×s | 457.77 | Joback Method |
| dvisc | 0.0003189 | Pa×s | 512.96 | Joback Method |
| dvisc | 0.0001133 | Pa×s | 568.16 | Joback Method |
| dvisc | 0.0000483 | Pa×s | 623.36 | Joback Method |
| dvisc | 0.0000237 | Pa×s | 678.55 | Joback Method |
| dvisc | 0.0000129 | Pa×s | 733.74 | Joback Method |
| dvisc | 0.0000077 | Pa×s | 788.94 | Joback Method |
| hfust | 45.30 | kJ/mol | 387.50 | NIST Webbook |
| hfust | 49.40 | kJ/mol | 386.30 | NIST Webbook |
| sfust | 116.90 | J/mol×K | 387.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.53406e+01 |
| Coeff. B | -6.02945e+03 |
| Coeff. C | -1.26323e+02 |
| Temperature range (K), min. | 526.87 |
| Temperature range (K), max. | 727.52 |

# Sources

**Cheméo Relay (1.0):**

**Vaporization, fusion and sublimation enthalpies of the dicarboxylic acids from C4 to C14 and C16:** https://www.doi.org/10.1016/j.jct.2004.12.011

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|---|---|
| **Solubility of tridecanedioic acid in pure solvent systems: An experimental and computational study:** | https://www.doi.org/10.1016/j.jct.2015.05.026 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C505522&Units=SI |
| **Cheméo Relay (1.0, beta):** | |
| **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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **chs:** | Standard solid enthalpy of combustion |
| **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 |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |