# 2,11-Dodecanediol, 2,11-dimethyl-

**Inchi:** InChI=1S/C14H30O2/c1-13(2,15)11-9-7-5-6-8-10-12-14(3,4)16/h15-16H,5-12H2,1-4H3
**InchiKey:** KKADLXHVRDQAFN-UHFFFAOYSA-N
**Formula:** C14H30O2
**SMILES:** CC(C)(O)CCCCCCCCC(C)(C)O
**Mol. weight [g/mol]:** 230.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.9530 | | Cheméo Relay (1.0) |
| chs | -8950.00 ± 4.00 | kJ/mol | NIST Webbook |
| hf | -695.03 | kJ/mol | Cheméo Relay (1.0) |
| hfs | -846.00 ± 4.00 | kJ/mol | NIST Webbook |
| hfus | 25.36 | kJ/mol | Joback Method |
| hvap | 107.34 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.62 | eV | Cheméo Relay (1.0) |
| log10ws | -3.81 | | Cheméo Relay (1.0) |
| logp | 3.649 | | Crippen Method |
| mcvol | 219.860 | ml/mol | McGowan Method |
| pc | 1826.28 | kPa | Joback Method |
| tb | 557.14 | K | Cheméo Relay (1.0) |
| tc | 742.56 | K | Cheméo Relay (1.0) |
| tf | 358.87 | K | Cheméo Relay (1.0) |
| vc | 0.874 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 657.66 | J/mol×K | 697.62 | Joback Method |
| cpg | 734.83 | J/mol×K | 867.72 | Joback Method |
| cpg | 723.48 | J/mol×K | 839.37 | Joback Method |
| cpg | 711.58 | J/mol×K | 811.02 | Joback Method |
| cpg | 699.09 | J/mol×K | 782.67 | Joback Method |
| cpg | 685.97 | J/mol×K | 754.32 | Joback Method |
| cpg | 672.17 | J/mol×K | 725.97 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000849 | Pa×s | 535.82 | Joback Method |
| dvisc | 0.0000077 | Pa×s | 697.62 | Joback Method |
| dvisc | 0.0000150 | Pa×s | 643.69 | Joback Method |
| dvisc | 0.0000329 | Pa×s | 589.75 | Joback Method |
| dvisc | 0.0074894 | Pa×s | 374.02 | Joback Method |
| dvisc | 0.0002705 | Pa×s | 481.89 | Joback Method |
| dvisc | 0.0011546 | Pa×s | 427.95 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C22092597&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **af:** | Acentric Factor |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |