# Propanoic acid, undecyl ester

**Inchi:** InChI=1S/C14H28O2/c1-3-5-6-7-8-9-10-11-12-13-16-14(15)4-2/h3-13H2,1-2H3
**InchiKey:** YYOMLCJPYHLLRY-UHFFFAOYSA-N
**Formula:** C14H28O2
**SMILES:** CCCCCCCCCCCOC(=O)CC
**Mol. weight [g/mol]:** 228.37

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -166.92 | kJ/mol | Joback Method |
| hf | -577.09 | kJ/mol | Joback Method |
| hfus | 34.80 | kJ/mol | Joback Method |
| hvap | 55.91 | kJ/mol | Joback Method |
| log10ws | -4.55 | | Crippen Method |
| logp | 4.470 | | Crippen Method |
| mcvol | 215.560 | ml/mol | McGowan Method |
| pc | 1579.71 | kPa | Joback Method |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1578.00 | | NIST Webbook |
| rinpol | 1577.00 | | NIST Webbook |
| rinpol | 1576.00 | | NIST Webbook |
| rinpol | 1564.00 | | NIST Webbook |
| rinpol | 1572.00 | | NIST Webbook |
| rinpol | 1575.00 | | NIST Webbook |
| rinpol | 1575.00 | | NIST Webbook |
| rinpol | 1564.00 | | NIST Webbook |
| rinpol | 1581.00 | | NIST Webbook |
| ripol | 1861.00 | | NIST Webbook |
| ripol | 1831.00 | | NIST Webbook |
| ripol | 1813.00 | | NIST Webbook |
| ripol | 1853.00 | | NIST Webbook |
| ripol | 1854.00 | | NIST Webbook |
| ripol | 1853.00 | | NIST Webbook |
| ripol | 1886.00 | | NIST Webbook |
| tb | 596.01 | K | Joback Method |
| tc | 764.02 | K | Joback Method |
| tf | 319.70 | K | Joback Method |
| vc | 0.844 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 567.02 | J/mol×K | 596.01 | Joback Method |
| cpg | 644.71 | J/mol×K | 736.02 | Joback Method |
| cpg | 630.49 | J/mol×K | 708.02 | Joback Method |
| cpg | 615.63 | J/mol×K | 680.02 | Joback Method |
| cpg | 600.10 | J/mol×K | 652.01 | Joback Method |
| cpg | 583.90 | J/mol×K | 624.01 | Joback Method |
| cpg | 658.29 | J/mol×K | 764.02 | Joback Method |
| dvisc | 0.0001532 | Pa×s | 596.01 | Joback Method |
| dvisc | 0.0002029 | Pa×s | 549.96 | Joback Method |
| dvisc | 0.0002827 | Pa×s | 503.91 | Joback Method |
| dvisc | 0.0004212 | Pa×s | 457.86 | Joback Method |
| dvisc | 0.0006860 | Pa×s | 411.80 | Joback Method |
| dvisc | 0.0012632 | Pa×s | 365.75 | Joback Method |
| dvisc | 0.0027735 | Pa×s | 319.70 | Joback Method |

# Sources

**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=R23885&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical 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 |