# Decanoic acid, propyl ester

**Other names:** Propyl caprate
Propyl decanoate
n-Propyl decanoate
**Inchi:** InChI=1S/C13H26O2/c1-3-5-6-7-8-9-10-11-13(14)15-12-4-2/h3-12H2,1-2H3
**InchiKey:** OVFMRFMJVFDSAA-UHFFFAOYSA-N
**Formula:** C13H26O2
**SMILES:** CCCCCCCCCC(=O)OCCC
**Mol. weight [g/mol]:** 214.34
**CAS:** 30673-60-0

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -175.34 | kJ/mol | Joback Method |
| hf | -556.45 | kJ/mol | Joback Method |
| hfus | 32.21 | kJ/mol | Joback Method |
| hvap | 53.69 | kJ/mol | Joback Method |
| log10ws | -4.13 | | Crippen Method |
| logp | 4.080 | | Crippen Method |
| mcvol | 201.470 | ml/mol | McGowan Method |
| pc | 1707.53 | kPa | Joback Method |
| rinpol | 1489.00 | | NIST Webbook |
| rinpol | 1476.00 | | NIST Webbook |
| rinpol | 1493.00 | | NIST Webbook |
| rinpol | 1487.00 | | NIST Webbook |
| rinpol | 1491.00 | | NIST Webbook |
| rinpol | 1489.00 | | NIST Webbook |
| rinpol | 1472.00 | | NIST Webbook |
| rinpol | 1493.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| rinpol | 1494.00 | | NIST Webbook |
| rinpol | 1473.00 | | NIST Webbook |
| rinpol | 1489.00 | | NIST Webbook |
| rinpol | 1473.00 | | NIST Webbook |
| ripol | 1720.00 | | NIST Webbook |
| ripol | 1729.00 | | NIST Webbook |
| ripol | 1697.00 | | NIST Webbook |
| ripol | 1726.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1743.00 | | NIST Webbook |
| ripol | 1720.00 | | NIST Webbook |
| ripol | 1722.00 | | NIST Webbook |
| ripol | 1725.00 | | NIST Webbook |
| ripol | 1720.00 | | NIST Webbook |
| tb | 573.13 | K | Joback Method |
| tc | 741.92 | K | Joback Method |
| tf | 308.43 | K | Joback Method |
| vc | 0.787 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 603.14 | J/mol×K | 741.92 | Joback Method |
| cpg | 589.97 | J/mol×K | 713.79 | Joback Method |
| cpg | 576.19 | J/mol×K | 685.66 | Joback Method |
| cpg | 561.79 | J/mol×K | 657.52 | Joback Method |
| cpg | 546.77 | J/mol×K | 629.39 | Joback Method |
| cpg | 531.11 | J/mol×K | 601.26 | Joback Method |
| cpg | 514.80 | J/mol×K | 573.13 | Joback Method |
| dvisc | 0.0029408 | Pa×s | 308.43 | Joback Method |
| dvisc | 0.0001702 | Pa×s | 573.13 | Joback Method |
| dvisc | 0.0002245 | Pa×s | 529.01 | Joback Method |
| dvisc | 0.0003115 | Pa×s | 484.90 | Joback Method |
| dvisc | 0.0004613 | Pa×s | 440.78 | Joback Method |
| dvisc | 0.0007456 | Pa×s | 396.66 | Joback Method |
| dvisc | 0.0013589 | Pa×s | 352.55 | Joback Method |
| hvapt | 62.40 | kJ/mol | 414.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.57945e+01 |
| Coeff. B | -4.89516e+03 |
| Coeff. C | -8.96440e+01 |
| Temperature range (K), min. | 405.32 |

| | |
|---|---|
| Temperature range (K), max. | 556.60 |

# Sources

| | |
|---|---|
| **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=C30673600&Units=SI |
| **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 |

# 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 |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **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 |