# 2,6-dipropylphenol

**Inchi:** InChI=1S/C12H18O/c1-3-6-10-8-5-9-11(7-4-2)12(10)13/h5,8-9,13H,3-4,6-7H2,1-2H3
**InchiKey:** NAILKKRDWBJCNH-UHFFFAOYSA-N
**Formula:** C12H18O
**SMILES:** CCCc1cccc(CCC)c1O
**Mol. weight [g/mol]:** 178.28
**CAS:** 6626-32-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.6597 | | Cheméo Relay (1.0) |
| gf | -1.68 | kJ/mol | Joback Method |
| hf | -228.74 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 26.27 | kJ/mol | Joback Method |
| hvap | 80.28 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.10 | eV | Cheméo Relay (1.0) |
| log10ws | -3.30 | | Cheméo Relay (1.0) |
| logp | 3.297 | | Crippen Method |
| mcvol | 162.050 | ml/mol | McGowan Method |
| pc | 2755.56 | kPa | Joback Method |
| tb | 526.16 | K | Cheméo Relay (1.0) |
| tc | 742.49 | K | Cheméo Relay (1.0) |
| tf | 307.65 | K | Cheméo Relay (1.0) |
| vc | 0.589 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 405.01 | J/mol×K | 586.24 | Joback Method |
| cpg | 420.01 | J/mol×K | 621.59 | Joback Method |
| cpg | 434.12 | J/mol×K | 656.94 | Joback Method |
| cpg | 447.42 | J/mol×K | 692.29 | Joback Method |
| cpg | 459.97 | J/mol×K | 727.64 | Joback Method |
| cpg | 471.84 | J/mol×K | 762.99 | Joback Method |
| cpg | 483.11 | J/mol×K | 798.34 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0015633 | Pa×s | 375.66 | Joback Method |
| dvisc | 0.0006387 | Pa×s | 410.76 | Joback Method |
| dvisc | 0.0003005 | Pa×s | 445.85 | Joback Method |
| dvisc | 0.0001578 | Pa×s | 480.95 | Joback Method |
| dvisc | 0.0000904 | Pa×s | 516.05 | Joback Method |
| dvisc | 0.0000557 | Pa×s | 551.14 | Joback Method |
| dvisc | 0.0000363 | Pa×s | 586.24 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.43403e+01 |
| Coeff. B | -4.42755e+03 |
| Coeff. C | -8.82540e+01 |
| Temperature range (K), min. | 361.81 |
| Temperature range (K), max. | 578.63 |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**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):**

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

# Legend

**af:** Acentric Factor

**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 |
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |