# 1,4-Dimethyl-2-propylbenzene

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|---|---|
| **Other names:** | 1,4-Dimethyl,2-n-Propylbenzene |
| | 1-propyl-2,5-dimethylbenzene |
| | Benzene, 1,4-dimethyl-2-propyl- |
| **Inchi:** | InChI=1S/C11H16/c1-4-5-11-8-9(2)6-7-10(11)3/h6-8H,4-5H2,1-3H3 |
| **InchiKey:** | PWEDYOIWLPZSRP-UHFFFAOYSA-N |
| **Formula:** | C11H16 |
| **SMILES:** | CCCc1cc(C)ccc1C |
| **Mol. weight [g/mol]:** | 148.24 |
| **CAS:** | 3042-50-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 134.89 | kJ/mol | Joback Method |
| hf | -56.78 | kJ/mol | Joback Method |
| hfus | 17.51 | kJ/mol | Joback Method |
| hvap | 43.68 | kJ/mol | Joback Method |
| log10ws | -3.64 | | Crippen Method |
| logp | 3.256 | | Crippen Method |
| mcvol | 142.090 | ml/mol | McGowan Method |
| pc | 2568.89 | kPa | Joback Method |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1148.00 | | NIST Webbook |
| rinpol | 1145.00 | | NIST Webbook |
| rinpol | 1148.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1148.00 | | NIST Webbook |
| rinpol | 1148.00 | | NIST Webbook |
| rinpol | 1148.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1386.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1415.00 | | NIST Webbook |
| ripol | 1385.90 | | NIST Webbook |
| ripol | 1425.00 | | NIST Webbook |
| ripol | 1425.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1438.00 | | NIST Webbook |
| ripol | 1452.00 | | NIST Webbook |
| ripol | 1413.00 | | NIST Webbook |
| ripol | 1386.00 | | NIST Webbook |
| tb | 480.00 ± 6.00 | K | NIST Webbook |
| tc | 692.15 | K | Joback Method |
| tf | 265.19 | K | Joback Method |
| vc | 0.543 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 301.47 | J/mol×K | 487.72 | Joback Method |
| cpg | 316.73 | J/mol×K | 521.79 | Joback Method |
| cpg | 331.23 | J/mol×K | 555.86 | Joback Method |
| cpg | 345.01 | J/mol×K | 589.93 | Joback Method |
| cpg | 358.09 | J/mol×K | 624.00 | Joback Method |
| cpg | 370.48 | J/mol×K | 658.08 | Joback Method |
| cpg | 382.22 | J/mol×K | 692.15 | Joback Method |
| dvisc | 0.0018138 | Pa×s | 265.19 | Joback Method |
| dvisc | 0.0010046 | Pa×s | 302.28 | Joback Method |
| dvisc | 0.0006331 | Pa×s | 339.37 | Joback Method |
| dvisc | 0.0004370 | Pa×s | 376.46 | Joback Method |
| dvisc | 0.0003223 | Pa×s | 413.54 | Joback Method |
| dvisc | 0.0002500 | Pa×s | 450.63 | Joback Method |
| dvisc | 0.0002015 | Pa×s | 487.72 | Joback Method |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

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

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol689.mol

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3042500&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 |
| **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 |