# Benzene, 1,2-dimethyl-4-(1-methylethyl)-

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|---|---|
| **Other names:** | 1,2-Dimethyl-4-isopropylbenzene |
| | 4-isopropyl-1,2-dimethyl-benzene |
| | Benzene, 1,2-dimethyl-4-isopropyl |
| **Inchi:** | InChI=1S/C11H16/c1-8(2)11-6-5-9(3)10(4)7-11/h5-8H,1-4H3 |
| **InchiKey:** | MGMSKQZIAGFMRU-UHFFFAOYSA-N |
| **Formula:** | C11H16 |
| **SMILES:** | Cc1ccc(C(C)C)cc1C |
| **Mol. weight [g/mol]:** | 148.24 |
| **CAS:** | 4132-77-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 132.45 | kJ/mol | Joback Method |
| hf | -62.06 | kJ/mol | Joback Method |
| hfus | 13.99 | kJ/mol | Joback Method |
| hvap | 43.29 | kJ/mol | Joback Method |
| log10ws | -3.61 | | Crippen Method |
| logp | 3.427 | | Crippen Method |
| mcvol | 142.090 | ml/mol | McGowan Method |
| pc | 2589.85 | kPa | Joback Method |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1120.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1140.00 | | NIST Webbook |
| rinpol | 1139.00 | | NIST Webbook |
| rinpol | 1117.50 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| rinpol | 1130.00 | | NIST Webbook |
| ripol | 1372.00 | | NIST Webbook |
| ripol | 1372.00 | | NIST Webbook |
| ripol | 1399.00 | | NIST Webbook |
| ripol | 1450.00 | | NIST Webbook |
| ripol | 1435.00 | | NIST Webbook |
| ripol | 1423.00 | | NIST Webbook |
| ripol | 1412.00 | | NIST Webbook |

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|---|---|---|---|
| ripol | 1411.00 | | NIST Webbook |
| ripol | 1372.50 | | NIST Webbook |
| tb | 473.00 ± 5.00 | K | NIST Webbook |
| tc | 696.41 | K | Joback Method |
| tf | 250.19 | K | Joback Method |
| vc | 0.537 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 301.65 | J/mol×K | 487.28 | Joback Method |
| cpg | 317.34 | J/mol×K | 522.13 | Joback Method |
| cpg | 332.23 | J/mol×K | 556.99 | Joback Method |
| cpg | 346.36 | J/mol×K | 591.84 | Joback Method |
| cpg | 359.74 | J/mol×K | 626.70 | Joback Method |
| cpg | 372.40 | J/mol×K | 661.55 | Joback Method |
| cpg | 384.36 | J/mol×K | 696.41 | Joback Method |
| dvisc | 0.0024629 | Pa×s | 250.19 | Joback Method |
| dvisc | 0.0012026 | Pa×s | 289.70 | Joback Method |
| dvisc | 0.0006975 | Pa×s | 329.22 | Joback Method |
| dvisc | 0.0004546 | Pa×s | 368.74 | Joback Method |
| dvisc | 0.0003219 | Pa×s | 408.25 | Joback Method |
| dvisc | 0.0002423 | Pa×s | 447.76 | Joback Method |
| dvisc | 0.0001909 | Pa×s | 487.28 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42585e+01 |
| Coeff. B | -3.87977e+03 |
| Coeff. C | -7.24920e+01 |
| Temperature range (K), min. | 350.20 |
| Temperature range (K), max. | 506.13 |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4132778&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 |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |
| **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 |