# 2-tert-butyl-4,5-dimethylphenol

**Inchi:** InChI=1S/C12H18O/c1-8-6-10(12(3,4)5)11(13)7-9(8)2/h6-7,13H,1-5H3
**InchiKey:** GDGFDAKCWRGGHW-UHFFFAOYSA-N
**Formula:** C12H18O
**SMILES:** Cc1cc(O)c(C(C)(C)C)cc1C
**Mol. weight [g/mol]:** 178.28
**CAS:** 1445-23-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -246.27 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 18.47 | kJ/mol | Joback Method |
| hvap | 74.46 | kJ/mol | Cheméo Relay (1.0) |
| ie | 7.81 | eV | Cheméo Relay (1.0) |
| logp | 3.307 | | Crippen Method |
| mcvol | 162.050 | ml/mol | McGowan Method |
| tb | 535.60 | K | Cheméo Relay (1.0) |
| tf | 366.17 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 407.95 | J/mol×K | 587.99 | Joback Method |
| cpg | 423.54 | J/mol×K | 625.70 | Joback Method |
| cpg | 438.08 | J/mol×K | 663.41 | Joback Method |
| cpg | 451.67 | J/mol×K | 701.12 | Joback Method |
| cpg | 464.42 | J/mol×K | 738.83 | Joback Method |
| cpg | 476.42 | J/mol×K | 776.54 | Joback Method |
| cpg | 487.78 | J/mol×K | 814.25 | Joback Method |
| dvisc | 0.0010949 | Pa×s | 390.60 | Joback Method |
| dvisc | 0.0004821 | Pa×s | 423.50 | Joback Method |
| dvisc | 0.0002389 | Pa×s | 456.40 | Joback Method |
| dvisc | 0.0001301 | Pa×s | 489.30 | Joback Method |
| dvisc | 0.0000765 | Pa×s | 522.19 | Joback Method |
| dvisc | 0.0000479 | Pa×s | 555.09 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000316 | Pa×s | 587.99 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.53068e+01 |
| Coeff. B | -4.75163e+03 |
| Coeff. C | -8.89490e+01 |
| Temperature range (K), min. | 405.32 |
| Temperature range (K), max. | 564.34 |

# Sources

**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

**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

# Legend

**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**hf:** Enthalpy of formation at standard conditions
**hfus:** Enthalpy of fusion at standard conditions
**hvap:** Enthalpy of vaporization at standard conditions
**ie:** Ionization energy
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume
**pvap:** Vapor pressure
**tb:** Normal Boiling Point Temperature

**tf:** Normal melting (fusion) point