# Phenol, 2,3,6-trimethyl-

**Other names:** 1-Hydroxy-2,3,6-trimethylbenzene
2,3,6-Trimethylphenol
**Inchi:** InChI=1S/C9H12O/c1-6-4-5-7(2)9(10)8(6)3/h4-5,10H,1-3H3
**InchiKey:** QQOMQLYQAXGHSU-UHFFFAOYSA-N
**Formula:** C9H12O
**SMILES:** Cc1ccc(C)c(O)c1C
**Mol. weight [g/mol]:** 136.19
**CAS:** 2416-94-6

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -36.57 | kJ/mol | Joback Method |
| hf | -192.81 | kJ/mol | Joback Method |
| hfus | 18.11 | kJ/mol | Joback Method |
| hsub | 86.70 ± 0.60 | kJ/mol | NIST Webbook |
| hvap | 52.24 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.317 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3754.57 | kPa | Joback Method |
| rinpol | 1198.00 | | NIST Webbook |
| rinpol | 1201.00 | | NIST Webbook |
| rinpol | 1203.00 | | NIST Webbook |
| rinpol | 1201.00 | | NIST Webbook |
| rinpol | 1241.90 | | NIST Webbook |
| rinpol | 1245.70 | | NIST Webbook |
| rinpol | 1239.30 | | NIST Webbook |
| ripol | 2028.00 | | NIST Webbook |
| ripol | 2039.00 | | NIST Webbook |
| ripol | 2031.00 | | NIST Webbook |
| tb | 522.58 | K | Joback Method |
| tc | 747.15 | K | Joback Method |
| tf | 354.65 ± 0.40 | K | NIST Webbook |
| tf | 335.45 ± 1.00 | K | NIST Webbook |
| tf | 335.15 ± 2.00 | K | NIST Webbook |
| tf | 335.00 ± 2.00 | K | NIST Webbook |
| vc | 0.398 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 329.50 | J/mol×K | 747.15 | Joback Method |
| cpg | 266.77 | J/mol×K | 522.58 | Joback Method |
| cpg | 278.94 | J/mol×K | 560.01 | Joback Method |
| cpg | 290.34 | J/mol×K | 597.44 | Joback Method |
| cpg | 301.03 | J/mol×K | 634.86 | Joback Method |
| cpg | 311.07 | J/mol×K | 672.29 | Joback Method |
| cpg | 320.54 | J/mol×K | 709.72 | Joback Method |
| dvisc | 0.0000662 | Pa×s | 522.58 | Joback Method |
| dvisc | 0.0017439 | Pa×s | 354.37 | Joback Method |
| dvisc | 0.0008278 | Pa×s | 382.40 | Joback Method |
| dvisc | 0.0004351 | Pa×s | 410.44 | Joback Method |
| dvisc | 0.0002482 | Pa×s | 438.47 | Joback Method |
| dvisc | 0.0001515 | Pa×s | 466.51 | Joback Method |
| dvisc | 0.0000978 | Pa×s | 494.54 | Joback Method |
| hfust | 22.05 | kJ/mol | 331.20 | NIST Webbook |
| hvapt | 51.10 ± 0.20 | kJ/mol | 431.00 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.67655e+01 |
| Coeff. B | -5.02691e+03 |
| Coeff. C | -8.29300e+01 |
| Temperature range (K), min. | 388.00 |
| Temperature range (K), max. | 521.81 |

# Sources

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

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2416946&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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hsub:** | Enthalpy of sublimation 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 |