# Phenol, 3-ethyl-4-methyl-

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|---|---|
| **Other names:** | 3-ethyl-p-cresol |
| | 3-ethyl-4-methylphenol |
| **Inchi:** | InChI=1S/C9H12O/c1-3-8-6-9(10)5-4-7(8)2/h4-6,10H,3H2,1-2H3 |
| **InchiKey:** | BTRPJOHXPQOVLS-UHFFFAOYSA-N |
| **Formula:** | C9H12O |
| **SMILES:** | CCc1cc(O)ccc1C |
| **Mol. weight [g/mol]:** | 136.19 |
| **CAS:** | 6161-67-7 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -26.94 | kJ/mol | Joback Method |
| hf | -181.34 | kJ/mol | Joback Method |
| hfus | 18.50 | kJ/mol | Joback Method |
| hvap | 51.58 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 2.263 | | Crippen Method |
| mcvol | 119.780 | ml/mol | McGowan Method |
| pc | 3824.55 | kPa | Joback Method |
| tb | 507.65 ± 3.00 | K | NIST Webbook |
| tb | 507.65 ± 3.00 | K | NIST Webbook |
| tb | 513.15 ± 4.00 | K | NIST Webbook |
| tc | 740.98 | K | Joback Method |
| tf | 306.15 ± 3.00 | K | NIST Webbook |
| tf | 306.15 ± 3.00 | K | NIST Webbook |
| vc | 0.398 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 267.07 | J/mol×K | 517.60 | Joback Method |
| cpg | 322.10 | J/mol×K | 703.75 | Joback Method |
| cpg | 312.50 | J/mol×K | 666.52 | Joback Method |
| cpg | 302.26 | J/mol×K | 629.29 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 291.33 | J/mol×K | 592.06 | Joback Method |
| cpg | 279.62 | J/mol×K | 554.83 | Joback Method |
| cpg | 331.15 | J/mol×K | 740.98 | Joback Method |
| dvisc | 0.0000711 | Pa×s | 517.60 | Joback Method |
| dvisc | 0.0001085 | Pa×s | 488.31 | Joback Method |
| dvisc | 0.0001750 | Pa×s | 459.02 | Joback Method |
| dvisc | 0.0003010 | Pa×s | 429.73 | Joback Method |
| dvisc | 0.0005605 | Pa×s | 400.43 | Joback Method |
| dvisc | 0.0011514 | Pa×s | 371.14 | Joback Method |
| dvisc | 0.0026759 | Pa×s | 341.85 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6161677&Units=SI |

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

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