# Phenol, 3-methyl-5-(1-methylethyl)-

**Other names:** 3-isopropyl-5-methyl phenol
Phenol, 3-methyl-5-(1-methylethyl)-
5-isopropyl-m-cresol
**Inchi:** InChI=1S/C10H14O/c1-7(2)9-4-8(3)5-10(11)6-9/h4-7,11H,1-3H3
**InchiKey:** ZDUIHRJGDMTBEX-UHFFFAOYSA-N
**Formula:** C10H14O
**SMILES:** Cc1cc(O)cc(C(C)C)c1
**Mol. weight [g/mol]:** 150.22

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5471 | | Cheméo Relay (1.0) |
| chs | -5636.00 | kJ/mol | NIST Webbook |
| hf | -210.10 | kJ/mol | NIST Webbook |
| hfs | -300.00 | kJ/mol | NIST Webbook |
| hfus | 17.57 | kJ/mol | Joback Method |
| hsub | 91.13 | kJ/mol | NIST Webbook |
| hsub | 89.90 | kJ/mol | NIST Webbook |
| hvap | 74.78 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.32 | eV | Cheméo Relay (1.0) |
| log10ws | -2.52 | | Cheméo Relay (1.0) |
| logp | 2.824 | | Crippen Method |
| mcvol | 133.870 | ml/mol | McGowan Method |
| pc | 3439.94 | kPa | Joback Method |
| ripol | 2287.00 | | NIST Webbook |
| ripol | 2204.00 | | NIST Webbook |
| ripol | 2197.00 | | NIST Webbook |
| ripol | 2197.00 | | NIST Webbook |
| ripol | 2287.00 | | NIST Webbook |
| tb | 514.15 ± 4.00 | K | NIST Webbook |
| tb | 514.15 ± 5.00 | K | NIST Webbook |
| tb | 514.15 ± 4.00 | K | NIST Webbook |
| tb | 514.15 ± 4.00 | K | NIST Webbook |
| tb | 514.20 | K | NIST Webbook |
| tc | 730.98 | K | Cheméo Relay (1.0) |
| tf | 327.15 ± 3.00 | K | NIST Webbook |
| tf | 322.65 ± 2.00 | K | NIST Webbook |

| | | | |
|---|---|---|---|
| tf | 321.65 ± 2.00 | K | NIST Webbook |
| tf | 322.55 ± 2.00 | K | NIST Webbook |
| tf | 327.15 ± 3.00 | K | NIST Webbook |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 311.65 | J/mol×K | 540.04 | Joback Method |
| cpg | 325.50 | J/mol×K | 577.45 | Joback Method |
| cpg | 338.45 | J/mol×K | 614.86 | Joback Method |
| cpg | 350.56 | J/mol×K | 652.28 | Joback Method |
| cpg | 361.90 | J/mol×K | 689.69 | Joback Method |
| cpg | 372.56 | J/mol×K | 727.10 | Joback Method |
| cpg | 382.61 | J/mol×K | 764.51 | Joback Method |
| dvisc | 0.0035167 | Pa×s | 338.12 | Joback Method |
| dvisc | 0.0012767 | Pa×s | 371.77 | Joback Method |
| dvisc | 0.0005484 | Pa×s | 405.43 | Joback Method |
| dvisc | 0.0002681 | Pa×s | 439.08 | Joback Method |
| dvisc | 0.0001452 | Pa×s | 472.73 | Joback Method |
| dvisc | 0.0000853 | Pa×s | 506.39 | Joback Method |
| dvisc | 0.0000535 | Pa×s | 540.04 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 375.70 | K | 0.50 | NIST Webbook |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C3228033&Units=SI

**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

| | |
|---|---|
| **af:** | Acentric Factor |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |