

2,5-Dimethoxy-p-cymene

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| Other names: | Thymohydroquinone dimethyl ether p-2,5-Dimethoxycymene 2,5-Dimethoxycymene Thymohydroquinone methyl ether p-Cymene, 2,5-dimethoxy 2,5-Dimethoxy-4-isopropyltoluene |
| Inchi: | InChI=1S/C12H18O2/c1-8(2)10-7-11(13-4)9(3)6-12(10)14-5/h6-8H,1-5H3 |
| InchiKey: | VTRMVHBUTNPBTP-UHFFFAOYSA-N |
| Formula: | C12H18O2 |
| SMILES: | COc1cc(C(C)C)c(OC)cc1C |
| Mol. weight [g/mol]: | 194.27 |
| CAS: | 14753-08-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -78.76 | kJ/mol | Joback Method |
| hf | -358.61 | kJ/mol | Joback Method |
| hfus | 18.56 | kJ/mol | Joback Method |
| hvap | 51.00 | kJ/mol | Joback Method |
| log10ws | -3.37 | | Crippen Method |
| logp | 3.136 | | Crippen Method |
| mcvol | 167.920 | ml/mol | McGowan Method |
| pc | 2246.13 | kPa | Joback Method |
| rinpol | 1399.00 | | NIST Webbook |
| rinpol | 1421.50 | | NIST Webbook |
| rinpol | 1430.00 | | NIST Webbook |
| rinpol | 1421.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1420.00 | | NIST Webbook |
| rinpol | 1425.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1418.20 | | NIST Webbook |
| rinpol | 1430.00 | | NIST Webbook |
| rinpol | 1420.00 | | NIST Webbook |
| rinpol | 1415.00 | | NIST Webbook |
| rinpol | 1424.00 | | NIST Webbook |
| rinpol | 1422.00 | | NIST Webbook |

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|-------|---------|----------------------|---------------|
| ripol | 1423.00 | | NIST Webbook |
| ripol | 1417.00 | | NIST Webbook |
| ripol | 1407.00 | | NIST Webbook |
| ripol | 1423.00 | | NIST Webbook |
| ripol | 1424.00 | | NIST Webbook |
| ripol | 1852.00 | | NIST Webbook |
| ripol | 1918.00 | | NIST Webbook |
| ripol | 1878.00 | | NIST Webbook |
| ripol | 1878.00 | | NIST Webbook |
| ripol | 1878.00 | | NIST Webbook |
| ripol | 1878.00 | | NIST Webbook |
| ripol | 1885.00 | | NIST Webbook |
| ripol | 1866.00 | | NIST Webbook |
| ripol | 1873.00 | | NIST Webbook |
| ripol | 1852.00 | | NIST Webbook |
| ripol | 1885.00 | | NIST Webbook |
| tb | 559.98 | K | Joback Method |
| tc | 763.30 | K | Joback Method |
| tf | 318.44 | K | Joback Method |
| vc | 0.629 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 399.02 | J/molxK | 559.98 | Joback Method |
| cpg | 414.65 | J/molxK | 593.87 | Joback Method |
| cpg | 429.61 | J/molxK | 627.75 | Joback Method |
| cpg | 443.90 | J/molxK | 661.64 | Joback Method |
| cpg | 457.51 | J/molxK | 695.53 | Joback Method |
| cpg | 470.43 | J/molxK | 729.41 | Joback Method |
| cpg | 482.66 | J/molxK | 763.30 | Joback Method |
| dvisc | 0.0010723 | Paxs | 318.44 | Joback Method |
| dvisc | 0.0006097 | Paxs | 358.70 | Joback Method |
| dvisc | 0.0003885 | Paxs | 398.95 | Joback Method |
| dvisc | 0.0002689 | Paxs | 439.21 | Joback Method |
| dvisc | 0.0001979 | Paxs | 479.47 | Joback Method |
| dvisc | 0.0001528 | Paxs | 519.72 | Joback Method |
| dvisc | 0.0001224 | Paxs | 559.98 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C14753083&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| 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 |

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