

Benzene, 2-ethyl-1,4-dimethyl-

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| Other names: | 1,4-DIMETHYL-2-ETHYLBENZENE 2,5-Dimethylethylbenzene 2-Ethyl-1,4-dimethylbenzene 2-Ethyl-p-xylene p-Xylene, 2-ethyl- |
| Inchi: | InChI=1S/C10H14/c1-4-10-7-8(2)5-6-9(10)3/h5-7H,4H2,1-3H3 |
| InchiKey: | AXIUBBVSOWPLDA-UHFFFAOYSA-N |
| Formula: | C10H14 |
| SMILES: | CCc1cc(C)ccc1C |
| Mol. weight [g/mol]: | 134.22 |
| CAS: | 1758-88-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|-----------------|--------|----------------|
| af | 0.3600 | | KDB |
| chl | -5851.10 ± 1.10 | kJ/mol | NIST Webbook |
| chl | -5850.70 ± 2.60 | kJ/mol | NIST Webbook |
| gf | 126.47 | kJ/mol | Joback Method |
| hf | -36.14 | kJ/mol | Joback Method |
| hfl | -85.30 ± 2.60 | kJ/mol | NIST Webbook |
| hfl | -84.80 ± 1.20 | kJ/mol | NIST Webbook |
| hfus | 14.92 | kJ/mol | Joback Method |
| hvap | 52.60 | kJ/mol | NIST Webbook |
| log10ws | -3.23 | | Crippen Method |
| logp | 2.866 | | Crippen Method |
| mcvol | 128.000 | ml/mol | McGowan Method |
| pc | 2900.00 | kPa | KDB |
| rinpol | 1066.00 | | NIST Webbook |
| rinpol | 1068.00 | | NIST Webbook |
| rinpol | 1059.00 | | NIST Webbook |
| rinpol | 1077.00 | | NIST Webbook |
| rinpol | 1083.00 | | NIST Webbook |
| rinpol | 1063.00 | | NIST Webbook |
| rinpol | 1072.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |
| rinpol | 1051.00 | | NIST Webbook |
| rinpol | 1059.00 | | NIST Webbook |

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| rinpol | 1064.00 | NIST Webbook |
| rinpol | 1085.20 | NIST Webbook |
| rinpol | 1066.00 | NIST Webbook |
| rinpol | 1070.00 | NIST Webbook |
| rinpol | 1068.00 | NIST Webbook |
| rinpol | 1074.00 | NIST Webbook |
| rinpol | 1071.00 | NIST Webbook |
| rinpol | 1067.00 | NIST Webbook |
| rinpol | 1062.00 | NIST Webbook |
| rinpol | 1049.00 | NIST Webbook |
| rinpol | 1073.00 | NIST Webbook |
| rinpol | 1064.00 | NIST Webbook |
| rinpol | 1074.60 | NIST Webbook |
| rinpol | 1093.00 | NIST Webbook |
| rinpol | 1061.00 | NIST Webbook |
| rinpol | 1073.00 | NIST Webbook |
| rinpol | 1063.00 | NIST Webbook |
| rinpol | 1068.00 | NIST Webbook |
| rinpol | 1068.50 | NIST Webbook |
| rinpol | 1069.50 | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |
| rinpol | 1068.00 | NIST Webbook |
| rinpol | 1069.00 | NIST Webbook |
| rinpol | 1067.20 | NIST Webbook |
| rinpol | 1066.70 | NIST Webbook |
| rinpol | 1067.70 | NIST Webbook |
| rinpol | 1067.00 | NIST Webbook |
| rinpol | 1073.00 | NIST Webbook |
| rinpol | 1089.00 | NIST Webbook |
| rinpol | 1067.00 | NIST Webbook |
| rinpol | 1067.00 | NIST Webbook |
| rinpol | 1069.00 | NIST Webbook |
| rinpol | 1069.00 | NIST Webbook |
| rinpol | 1059.00 | NIST Webbook |
| rinpol | 1054.80 | NIST Webbook |
| rinpol | 1062.00 | NIST Webbook |
| rinpol | 1054.29 | NIST Webbook |
| rinpol | 1081.00 | NIST Webbook |
| rinpol | 1080.00 | NIST Webbook |
| rinpol | 1085.00 | NIST Webbook |
| rinpol | 1089.00 | NIST Webbook |
| rinpol | 1060.50 | NIST Webbook |
| rinpol | 1060.00 | NIST Webbook |

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|--------|---------------|----------------------|--------------|
| rinpol | 1086.90 | | NIST Webbook |
| rinpol | 1061.00 | | NIST Webbook |
| rinpol | 1090.00 | | NIST Webbook |
| rinpol | 1068.00 | | NIST Webbook |
| rinpol | 1067.00 | | NIST Webbook |
| rinpol | 1068.80 | | NIST Webbook |
| rinpol | 1059.60 | | NIST Webbook |
| rinpol | 1063.00 | | NIST Webbook |
| rinpol | 1062.00 | | NIST Webbook |
| rinpol | 1062.32 | | NIST Webbook |
| rinpol | 1063.12 | | NIST Webbook |
| rinpol | 1077.00 | | NIST Webbook |
| ripol | 1307.00 | | NIST Webbook |
| ripol | 1307.00 | | NIST Webbook |
| ripol | 1344.00 | | NIST Webbook |
| ripol | 1321.00 | | NIST Webbook |
| ripol | 1344.00 | | NIST Webbook |
| ripol | 1341.00 | | NIST Webbook |
| ripol | 1323.00 | | NIST Webbook |
| ripol | 1321.00 | | NIST Webbook |
| ripol | 1364.00 | | NIST Webbook |
| ripol | 1339.00 | | NIST Webbook |
| ripol | 1321.10 | | NIST Webbook |
| ripol | 1335.00 | | NIST Webbook |
| ripol | 1343.50 | | NIST Webbook |
| tb | 459.60 ± 0.30 | K | NIST Webbook |
| tb | 459.00 ± 3.00 | K | NIST Webbook |
| tb | 459.98 ± 0.20 | K | NIST Webbook |
| tb | 459.60 ± 0.30 | K | NIST Webbook |
| tb | 460.06 ± 0.20 | K | NIST Webbook |
| tb | 460.40 ± 2.00 | K | NIST Webbook |
| tb | 459.60 ± 0.15 | K | NIST Webbook |
| tb | 459.60 ± 1.00 | K | NIST Webbook |
| tb | 460.06 ± 0.20 | K | NIST Webbook |
| tb | 460.10 | K | KDB |
| tb | 459.60 ± 0.30 | K | NIST Webbook |
| tb | 461.70 ± 1.50 | K | NIST Webbook |
| tb | 460.10 | K | NIST Webbook |
| tc | 662.60 | K | KDB |
| tf | 219.50 | K | KDB |
| tf | 219.41 ± 0.20 | K | NIST Webbook |
| vc | 0.461 | m ³ /kmol | KDB |
| zc | 0.2425620 | | KDB |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 322.46 | J/molxK | 637.55 | Joback Method |
| cpg | 298.71 | J/molxK | 568.47 | Joback Method |
| cpg | 285.86 | J/molxK | 533.92 | Joback Method |
| cpg | 272.33 | J/molxK | 499.38 | Joback Method |
| cpg | 258.11 | J/molxK | 464.84 | Joback Method |
| cpg | 310.90 | J/molxK | 603.01 | Joback Method |
| cpg | 333.41 | J/molxK | 672.09 | Joback Method |
| dvisc | 0.0017125 | Paxs | 253.92 | Joback Method |
| dvisc | 0.0002068 | Paxs | 464.84 | Joback Method |
| dvisc | 0.0002547 | Paxs | 429.69 | Joback Method |
| dvisc | 0.0003255 | Paxs | 394.53 | Joback Method |
| dvisc | 0.0004364 | Paxs | 359.38 | Joback Method |
| dvisc | 0.0006236 | Paxs | 324.23 | Joback Method |
| dvisc | 0.0009718 | Paxs | 289.07 | Joback Method |
| hvapt | 48.00 | kJ/mol | 414.00 | NIST Webbook |
| hvapt | 48.70 | kJ/mol | 369.50 | NIST Webbook |
| rho | 872.44 | kg/m3 | 293.10 | KDB |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.47855e+01 |
| Coeff. B | -4.20569e+03 |
| Coeff. C | -4.63260e+01 |
| Temperature range (K), min. | 336.42 |
| Temperature range (K), max. | 490.24 |

| Information | Value |
|---------------|--|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$ |
| Coeff. A | 5.69470e+01 |
| Coeff. B | -7.63454e+03 |

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| Coeff. C | -5.89162e+00 |
| Coeff. D | 1.81744e-06 |
| Temperature range (K), min. | 219.52 |
| Temperature range (K), max. | 663.00 |

Sources

| | |
|---|---|
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| KDB Vapor Pressure Data: | https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=683 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| KDB: | https://www.thermo.com/files/research/kdb/mol/mol683.mol |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1758889&Units=SI |

Legend

| | |
|-----------------|---|
| af: | Acentric Factor |
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfl: | Liquid phase enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion 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 |
| rho: | Liquid Density |
| 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
zc: Critical Compressibility

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