

benzene, 1,2,3,5-tetraethyl-

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|-----------------------------|---|
| Other names: | 1,2,3,5-Tetraethylbenzene |
| Inchi: | InChI=1S/C14H22/c1-5-11-9-12(6-2)14(8-4)13(7-3)10-11/h9-10H,5-8H2,1-4H3 |
| InchiKey: | QJEXLOSCNXHBAX-UHFFFAOYSA-N |
| Formula: | C14H22 |
| SMILES: | CCc1cc(CC)c(CC)c(CC)c1 |
| Mol. weight [g/mol]: | 190.32 |
| CAS: | 38842-05-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|---------|----------------|
| gf | 150.52 | kJ/mol | Joback Method |
| hf | -130.17 | kJ/mol | Joback Method |
| hfus | 24.89 | kJ/mol | Joback Method |
| hvap | 51.02 | kJ/mol | Joback Method |
| log10ws | -4.68 | | Crippen Method |
| logp | 3.936 | | Crippen Method |
| mcvol | 184.360 | ml/mol | McGowan Method |
| pc | 1930.44 | kPa | Joback Method |
| rinpol | 1390.00 | | NIST Webbook |
| tb | 561.34 | K | Joback Method |
| tc | 758.43 | K | Joback Method |
| tf | 252.00 ± 2.00 | K | NIST Webbook |
| vc | 0.712 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 443.27 | J/molxK | 561.34 | Joback Method |
| cpg | 460.57 | J/molxK | 594.19 | Joback Method |
| cpg | 477.05 | J/molxK | 627.04 | Joback Method |
| cpg | 492.74 | J/molxK | 659.89 | Joback Method |
| cpg | 507.66 | J/molxK | 692.73 | Joback Method |
| cpg | 521.83 | J/molxK | 725.58 | Joback Method |
| cpg | 535.27 | J/molxK | 758.43 | Joback Method |

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|-------|-----------|--------|--------|---------------|
| dvisc | 0.0014453 | Paxs | 311.52 | Joback Method |
| dvisc | 0.0008167 | Paxs | 353.16 | Joback Method |
| dvisc | 0.0005205 | Paxs | 394.79 | Joback Method |
| dvisc | 0.0003615 | Paxs | 436.43 | Joback Method |
| dvisc | 0.0002676 | Paxs | 478.07 | Joback Method |
| dvisc | 0.0002078 | Paxs | 519.70 | Joback Method |
| dvisc | 0.0001675 | Paxs | 561.34 | Joback Method |
| hvapt | 64.80 | kJ/mol | 467.00 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.42717e+01 |
| Coeff. B | -4.62805e+03 |
| Coeff. C | -5.45830e+01 |
| Temperature range (K), min. | 385.53 |
| Temperature range (K), max. | 571.09 |

Sources

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|---|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C38842056&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/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| KDB: | https://www.cheric.org/files/research/kdb/mol/mol709.mol |

Legend

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|---------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |

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|-----------------|---|
| hf: | 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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