# Styrene

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|---|---|
| **Other names:** | Annamene |
| | Benzene, ethenyl- |
| | Benzene, vinyl- |
| | Bulstren K-525-19 |
| | Cinnamene |
| | Cinnamenol |
| | Cinnaminol |
| | Cinnamol |
| | Ethenylbenzene |
| | Ethylene, phenyl- |
| | NCI-C02200 |
| | NSC 62785 |
| | Phenethylene |
| | Phenylethene |
| | Phenylethylene |
| | Stirolo |
| | Styreen |
| | Styren |
| | Styrene monomer |
| | Styrol |
| | Styrol (German) |
| | Styrole |
| | Styrolene |
| | Styropol SO |
| | Vinylbenzen |
| | Vinylbenzene |
| | Vinylbenzene (styrene) |
| | Vinylbenzol |
| | ethenylbenzene (styrene) |
| **Inchi:** | InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2 |
| **InchiKey:** | PPBRXRYQALVLMV-UHFFFAOYSA-N |
| **Formula:** | C8H8 |
| **SMILES:** | C=Cc1ccccc1 |
| **Mol. weight [g/mol]:** | 104.15 |
| **CAS:** | 100-42-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 839.50 | kJ/mol | NIST Webbook |
| basg | 809.20 | kJ/mol | NIST Webbook |
| gf | 216.73 | kJ/mol | Joback Method |
| hf | 146.90 ± 1.00 | kJ/mol | NIST Webbook |
| hf | 151.50 | kJ/mol | NIST Webbook |
| hf | -15.10 | kJ/mol | NIST Webbook |
| hf | 131.50 ± 4.00 | kJ/mol | NIST Webbook |
| hfl | 108.00 | kJ/mol | NIST Webbook |
| hfl | 103.40 ± 0.92 | kJ/mol | NIST Webbook |
| hfl | -58.60 | kJ/mol | NIST Webbook |
| hfl | 87.60 ± 4.00 | kJ/mol | NIST Webbook |
| hfus | 9.24 | kJ/mol | Joback Method |
| hvap | 43.90 | kJ/mol | NIST Webbook |
| hvap | 43.93 ± 0.42 | kJ/mol | NIST Webbook |
| hvap | 43.50 ± 0.40 | kJ/mol | NIST Webbook |
| hvap | 43.20 | kJ/mol | NIST Webbook |
| hvap | 43.50 | kJ/mol | NIST Webbook |
| ie | 8.55 | eV | NIST Webbook |
| ie | 8.55 | eV | NIST Webbook |
| ie | 8.49 | eV | NIST Webbook |
| ie | 8.50 | eV | NIST Webbook |
| ie | 8.58 | eV | NIST Webbook |
| ie | 8.48 | eV | NIST Webbook |
| ie | 8.47 ± 0.02 | eV | NIST Webbook |
| ie | 8.42 | eV | NIST Webbook |
| ie | 8.43 ± 0.01 | eV | NIST Webbook |
| ie | 8.53 | eV | NIST Webbook |
| ie | 8.20 ± 0.10 | eV | NIST Webbook |
| ie | 8.28 ± 0.04 | eV | NIST Webbook |
| ie | 8.43 | eV | NIST Webbook |
| ie | 8.47 | eV | NIST Webbook |
| ie | 8.46 ± 0.00 | eV | NIST Webbook |
| ie | 8.46 ± 0.00 | eV | NIST Webbook |
| ie | 8.42 | eV | NIST Webbook |
| ie | 8.40 ± 0.02 | eV | NIST Webbook |
| log10ws | -2.82 | | Estimated Solubility Method |
| log10ws | -2.70 | | Aqueous Solubility Prediction Method |
| logp | 2.330 | | Crippen Method |
| mcvol | 95.520 | ml/mol | McGowan Method |
| pc | 3843.54 | kPa | Joback Method |
| rinpol | 874.35 | | NIST Webbook |

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| rinpol | 872.00 | NIST Webbook |
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| rinpol | 890.50 | NIST Webbook |
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| rinpol | 874.70 | NIST Webbook |
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| rinpol | 874.90 | NIST Webbook |
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| rinpol | 873.00 | NIST Webbook |
| rinpol | 873.00 | NIST Webbook |
| rinpol | 862.00 | NIST Webbook |
| rinpol | 877.80 | NIST Webbook |
| ripol | 1251.00 | NIST Webbook |
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| ripol | 1263.00 | | NIST Webbook |
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| ripol | 1248.00 | | NIST Webbook |
| ripol | 1263.00 | | NIST Webbook |
| ripol | 1254.00 | | NIST Webbook |
| ripol | 1245.00 | | NIST Webbook |
| sg | 345.10 ± 2.10 | J/mol×K | NIST Webbook |
| sl | 237.60 | J/mol×K | NIST Webbook |
| sl | 237.57 | J/mol×K | NIST Webbook |
| sl | 240.50 | J/mol×K | NIST Webbook |
| tb | 405.80 | K | Joback Method |
| tc | 620.11 | K | Joback Method |
| tf | 204.58 | K | Joback Method |
| tt | 242.47 ± 0.10 | K | NIST Webbook |
| tt | 242.47 ± 0.10 | K | NIST Webbook |
| tt | 242.47 ± 0.07 | K | NIST Webbook |
| vc | 0.356 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| cpg | 151.29 ± 0.76 | J/mol×K | 373.15 | NIST Webbook |
| cpl | 183.20 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 235.60 | J/mol×K | 298.00 | NIST Webbook |
| cpl | 182.84 | J/mol×K | 298.15 | NIST Webbook |
| cpl | 179.90 | J/mol×K | 298.50 | NIST Webbook |
| cpl | 182.60 | J/mol×K | 298.16 | NIST Webbook |
| dvisc | 0.0004190 | Pa×s | 343.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0004620 | Pa×s | 333.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0003490 | Pa×s | 363.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0005130 | Pa×s | 323.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |

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|---|---|---|---|---|
| dvisc | 0.0005770 | Pa×s | 313.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0006540 | Pa×s | 303.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0006990 | Pa×s | 298.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0003810 | Pa×s | 353.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |
| dvisc | 0.0007490 | Pa×s | 293.15 | Densities and Viscosities of Binary Mixtures of Ethylbenzene + N-Methyl-2-pyrrolidone, Ethylbenzene + Sulfolane, and Styrene + Octane from (303.15 to 353.15) K and Atmospheric Pressure |

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|---|---|---|---|---|
| hfust | 10.96 | kJ/mol | 242.27 | NIST Webbook |
| hfust | 10.95 | kJ/mol | 242.47 | NIST Webbook |
| hfust | 10.95 | kJ/mol | 242.47 | NIST Webbook |
| hfust | 10.96 | kJ/mol | 242.30 | NIST Webbook |
| hfust | 10.95 | kJ/mol | 242.30 | NIST Webbook |
| hfust | 10.95 | kJ/mol | 242.27 | NIST Webbook |
| hvapt | 43.10 | kJ/mol | 360.00 | NIST Webbook |
| hvapt | 40.20 | kJ/mol | 347.50 | NIST Webbook |
| hvapt | 42.50 | kJ/mol | 319.50 | NIST Webbook |
| hvapt | 42.50 | kJ/mol | 289.50 | NIST Webbook |
| hvapt | 41.50 | kJ/mol | 376.50 | NIST Webbook |
| pvap | 20.00 | kPa | 366.20 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 25.00 | kPa | 372.40 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 22.50 | kPa | 369.40 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 17.50 | kPa | 362.60 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |

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| pvap | 15.00 | kPa | 358.50 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 12.50 | kPa | 353.90 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 10.00 | kPa | 348.30 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 7.50 | kPa | 341.40 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| pvap | 5.00 | kPa | 332.40 | Isobaric Low-Pressure Vapor Liquid Equilibrium Data for Ethylbenzene + Styrene + Sulfolane and the Three Constituent Binary Systems |
| rfi | 1.53520 | | 313.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.53210 | | 318.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |

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|---|---|---|---|
| rfi | 1.52910 | 323.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.54380 | 298.15 | Isobaric Vapor-Liquid Equilibria for the Binary Mixtures of Styrene with Ethylbenzene, o-Xylene, m-Xylene, and p-Xylene |
| rfi | 1.53800 | 308.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.54600 | 293.15 | Effect of temperature on the volumetric properties of (cyclohexanone + an aromatic hydrocarbon) |
| rfi | 1.54400 | 298.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.54600 | 293.15 | Experimental densities and excess volumes for binary mixtures of (dimethyl sulfoxide + an aromatic hydrocarbon) at temperatures from (293.15 to 353.15) K at atmospheric pressure |
| rfi | 1.55050 | 288.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |

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| rfi | 1.55330 | 283.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.54090 | 303.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rfi | 1.54660 | 298.15 | Effects of the presence of ethylacetate or benzene on the densities and volumetric properties of mixture (styrene + N,N-dimethylformamide) |
| rfi | 1.54600 | 298.15 | The volumetric properties of (1,2-propanediol carbonate + benzene, or toluene, or styrene) binary mixtures at temperatures from T = 293.15 K to T = 353.15 K |
| rfi | 1.54290 | 313.15 | Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures |
| rfi | 1.54370 | 308.15 | Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures |

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| rfi | 1.54560 | | 298.15 | Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures |
| rfi | 1.54600 | | 293.15 | A study of densities and volumetric properties of binary mixtures containing nitrobenzene at T = (293.15 to 353.15) K |
| rfi | 1.54450 | | 303.15 | Volumetric, Viscometric, Ultrasonic, and Refractive Index Properties of Liquid Mixtures of Benzene with Industrially Important Monomers at Different Temperatures |
| rfi | 1.54720 | | 293.15 | Solubilities of Diethyl Phthalate, Dicyclopentadiene, and Styrene in Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate |
| rhol | 897.39 | kg/m3 | 303.15 | Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K |

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| rhol | 901.94 | kg/m3 | 298.15 | Volumetric Properties of 3-Methylbutyl Ethanoate with Ethyl Acrylate, Butyl Acrylate, Methyl Methacrylate, and Styrene at 25 C |
| rhol | 888.47 | kg/m3 | 313.15 | Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K |
| rhol | 900.52 | kg/m3 | 298.15 | Separation of ethylbenzene/styrene systems using ionic liquids in ternary LLE |
| rhol | 906.26 | kg/m3 | 293.15 | Density, excess volume, and excess coefficient of thermal expansion of the binary systems of dimethyl carbonate with butyl methacrylate, allyl methacrylate, styrene, and vinyl acetate at T = (293.15, 303.15, and 313.15) K |
| sfust | 45.32 | J/mol×K | 242.27 | NIST Webbook |
| sfust | 45.16 | J/mol×K | 242.27 | NIST Webbook |
| sfust | 45.16 | J/mol×K | 242.47 | NIST Webbook |
| sfust | 45.20 | J/mol×K | 242.47 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|

| Property code | pvap |
|---|---|
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.39212e+01 |
| Coeff. B | -3.31078e+03 |
| Coeff. C | -6.31110e+01 |
| Temperature range (K), min. | 305.95 |
| Temperature range (K), max. | 447.65 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 8.60058e+01 |
| Coeff. B | -8.11907e+03 |
| Coeff. C | -1.04313e+01 |
| Coeff. D | 5.61169e-06 |
| Temperature range (K), min. | 242.54 |
| Temperature range (K), max. | 648.00 |

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| **KDB Pure (Kyushu Database of Physical Properties Database) Liquid Phase Chemical:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=718 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C100425&Units=SI |
| **Determination of the thermodynamic parameters of ionic liquid 1-propyl-3-methylimidazolium bromide by gas-liquid chromatography:** | https://www.doi.org/10.1016/j.jct.2018.09.023 |
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# Legend

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|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase 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 |
| **hfust:** | Enthalpy of fusion at a given temperature |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **hvapt:** | Enthalpy of vaporization at a given temperature |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |

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| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **rfi:** | Refractive Index |
| **rhol:** | Liquid Density |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **sfust:** | Entropy of fusion at a given temperature |
| **sg:** | Molar entropy at standard conditions |
| **sl:** | Liquid phase molar entropy at standard conditions |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |

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