# Benzene, (trifluoromethyl)-

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|---|---|
| **Other names:** | (Trifluoromethyl)benzene |
| | .alpha.,.alpha.,.alpha.-trifluorotoluene |
| | 1,1,1-TRIFLUOROTOLUENE |
| | ALPHA,ALPHA,ALPHA-TRIFLUOROTOLUENE |
| | BENZENYL FLUORIDE |
| | BENZOTRIFLUORIDE |
| | Benzylidyne fluoride |
| | Benzyltrifluoride |
| | NSC 8038 |
| | Phenylfluoroform |
| | Toluene, «alpha»,«alpha»,«alpha»-trifluoro- |
| | Toluene, Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-trifluoro- |
| | Trifluoro(phenyl)methane |
| | Trifluoromethylbenzene |
| | UN 2338 |
| | USAF MA-16 |
| | «alpha»,«alpha»,«alpha»-Trifluorotoluene |
| | Â«alphaÂ»,Â«alphaÂ»,Â«alphaÂ»-Trifluorotoluene |
| **Inchi:** | InChI=1S/C7H5F3/c8-7(9,10)6-4-2-1-3-5-6/h1-5H |
| **InchiKey:** | GETTZEONDQJALK-UHFFFAOYSA-N |
| **Formula:** | C7H5F3 |
| **SMILES:** | FC(F)(F)c1ccccc1 |
| **Mol. weight [g/mol]:** | 146.11 |
| **CAS:** | 98-08-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -3369.30 ± 0.50 | kJ/mol | NIST Webbook |
| chl | -3390.50 | kJ/mol | NIST Webbook |
| ea | 0.00 | eV | NIST Webbook |
| gf | -461.12 | kJ/mol | Joback Method |
| hf | -581.03 | kJ/mol | NIST Webbook |
| hfl | -620.45 | kJ/mol | NIST Webbook |
| hfus | 9.75 | kJ/mol | Joback Method |
| hvap | 37.10 | kJ/mol | NIST Webbook |
| hvap | 37.67 | kJ/mol | NIST Webbook |
| hvap | 37.60 | kJ/mol | NIST Webbook |

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|---|---|---|---|
| ie | 9.86 | eV | NIST Webbook |
| ie | 9.69 ± 0.00 | eV | NIST Webbook |
| ie | 9.69 ± 0.03 | eV | NIST Webbook |
| ie | 9.70 | eV | NIST Webbook |
| ie | 9.68 | eV | NIST Webbook |
| ie | 9.69 ± 0.01 | eV | NIST Webbook |
| ie | 9.69 ± 0.01 | eV | NIST Webbook |
| ie | 9.68 ± 0.02 | eV | NIST Webbook |
| log10ws | -2.51 | | Estimated Solubility Method |
| log10ws | -2.51 | | Aqueous Solubility Prediction Method |
| logp | 2.705 | | Crippen Method |
| mcvol | 91.040 | ml/mol | McGowan Method |
| pc | 3564.27 | kPa | Joback Method |
| rinpol | 700.00 | | NIST Webbook |
| rinpol | 656.30 | | NIST Webbook |
| rinpol | 656.40 | | NIST Webbook |
| rinpol | 696.00 | | NIST Webbook |
| sl | 271.50 | J/mol×K | NIST Webbook |
| tb | 374.50 ± 0.50 | K | NIST Webbook |
| tb | 375.20 | K | NIST Webbook |
| tb | 375.19 ± 0.20 | K | NIST Webbook |
| tb | 375.70 | K | Phase diagrams of (vapour + liquid) equilibrium for binary mixtures of a,a,a-trifluorotoluene with ethanol, or benzene, or chloroform at pressure 101.4 kPa |
| tb | 375.20 ± 0.40 | K | NIST Webbook |
| tb | 375.40 ± 1.00 | K | NIST Webbook |
| tb | 376.61 | K | KDB |
| tb | 375.00 | K | NIST Webbook |
| tb | 375.20 | K | NIST Webbook |
| tc | 559.90 | K | NIST Webbook |
| tf | 244.78 | K | Aqueous Solubility Prediction Method |
| tf | 244.00 ± 0.02 | K | NIST Webbook |
| tt | 244.14 ± 0.07 | K | NIST Webbook |
| tt | 244.14 ± 0.02 | K | NIST Webbook |
| vc | 0.362 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 205.09 | J/mol×K | 507.64 | Joback Method |
| cpg | 195.99 | J/mol×K | 475.93 | Joback Method |
| cpg | 186.19 | J/mol×K | 444.23 | Joback Method |
| cpg | 175.67 | J/mol×K | 412.52 | Joback Method |
| cpg | 221.37 | J/mol×K | 571.05 | Joback Method |
| cpg | 213.54 | J/mol×K | 539.34 | Joback Method |
| cpg | 164.39 | J/mol×K | 380.82 | Joback Method |
| cpl | 188.45 | J/mol×K | 298.15 | NIST Webbook |
| hfust | 11.99 | kJ/mol | 242.00 | NIST Webbook |
| hfust | 13.77 | kJ/mol | 244.00 | NIST Webbook |
| hfust | 13.78 | kJ/mol | 244.14 | NIST Webbook |
| hsubt | 54.40 | kJ/mol | 227.50 | NIST Webbook |
| hvapt | 35.60 | kJ/mol | 370.50 | NIST Webbook |
| hvapt | 38.50 | kJ/mol | 314.00 | NIST Webbook |
| hvapt | 32.63 | kJ/mol | 375.20 | NIST Webbook |
| hvapt | 39.10 | kJ/mol | 308.00 | NIST Webbook |
| hvapt | 32.60 ± 0.10 | kJ/mol | 375.00 | NIST Webbook |
| hvapt | 34.10 ± 0.10 | kJ/mol | 353.00 | NIST Webbook |
| hvapt | 35.40 ± 0.10 | kJ/mol | 334.00 | NIST Webbook |
| hvapt | 32.40 | kJ/mol | 495.00 | NIST Webbook |
| hvapt | 35.70 | kJ/mol | 370.50 | NIST Webbook |
| hvapt | 35.90 | kJ/mol | 353.50 | NIST Webbook |
| hvapt | 31.60 | kJ/mol | 500.00 | NIST Webbook |
| rfi | 1.41320 | | 298.15 | Study of Vapor-Liquid Equilibrium for Binary Mixtures (Chloroform + 2,2,2-Trifluoroethanol) and (r,r,r-Trifluorotoluene + 2,2,2-Trifluoroethanol) at Pressure 102 kPa |

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|---|---|---|---|---|
| rhol | 1182.18 | kg/m3 | 298.15 | Volumetric properties of binary and ternary mixtures of diisopropyl ether, a,a,a-trifluorotoluene, 2,2,2-trifluoroethanol, and ethanol at a temperature 298.15 K and pressure 101 kPa |
| sfust | 56.45 | J/mol×K | 244.14 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.42129e+01 |
| Coeff. B | -3.14473e+03 |
| Coeff. C | -4.72370e+01 |
| Temperature range (K), min. | 244.14 |
| Temperature range (K), max. | 400.52 |

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/T + C*ln(T) + D*T^2 |
| Coeff. A | 5.19443e+01 |
| Coeff. B | -5.93323e+03 |
| Coeff. C | -5.37094e+00 |
| Coeff. D | 2.26368e-06 |
| Temperature range (K), min. | 244.14 |
| Temperature range (K), max. | 565.00 |

# Sources

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|---|---|
| **KDB Pure (Korean Thermophysical Properties Databank):** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1694 |
| **KDB:** | https://www.cheric.org/files/research/kdb/mol/mol1694.mol |
| **Estimated Solubility Method:** | http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt |
| **Study of Vapor-Liquid Equilibrium for Binary Mixtures (Chloroform + 2,2,2-Trifluoroethanol) and (r,r,r-Trifluorotoluene + 2,2,2-Trifluoroethanol) at Pressure 102 kPa:** | https://www.doi.org/10.1021/je700103k |

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **KDB Vapor Pressure Data:** | https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1694 |
| **Solubilities and Phase Equilibria for Ternary Solutions of alpha, alpha, alpha-Trifluorotoluene, Water, and 2-Propanol at Three Temperatures and Pressure of 101.2 kPa:** | https://www.doi.org/10.1021/je600526x |
| **Volumetric properties of binary and ternary mixtures of diisopropyl ether, 2,2,2-trifluoroethanol, and ethanol at a temperature 298.15 K and pressure 101 kPa:** | https://www.doi.org/10.1016/j.jct.2006.09.006 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Solubilities and liquid liquid equilibria of (water + ethanol + α,α,α-trifluorotoluene) at temperatures T = (288.15, 298.15, and 308.15) K and pressure p = 101.2 kPa:** | https://www.doi.org/10.1016/j.jct.2006.09.004 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Phase diagrams of (vapour + liquid) equilibrium for binary mixtures of α,α,α-trifluorotoluene with ethanol, or benzene, or chloroform at pressure 101.4 kPa:** | https://www.doi.org/10.1016/j.jct.2007.09.002 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C98088&Units=SI |
| **Aqueous Solubility Prediction Method:** | http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa |

# Legend

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|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **ea:** | Electron affinity |
| **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 |
| **hsubt:** | Enthalpy of sublimation 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 |
| **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 |
| **sfust:** | Entropy of fusion at a given temperature |
| **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