# Ethane, 1,1,1-trichloro-2,2,2-trifluoro-

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|---|---|
| **Other names:** | 1,1,1-Trichloro-2,2,2-trifluoroethane |
| | 1,1,1-Trichlorotrifluoroethane |
| | 1,1,1-Trifluoro-2,2,2-trichloroethane |
| | 1,1,1-Trifluorotrichloroethane |
| | 2,2,2-Trichloro-1,1,1-trifluoro-ethane |
| | CF3CCl3 |
| | CFC 113a |
| | F 113a |
| | FC 113a |
| | Freon FT |
| | Freon-FT |
| | Precision cleaning agent |
| | R-113a |
| | T-WD602 |
| | Trichlorotrifluoroethane |
| | freon 113a |
| **Inchi:** | InChI=1S/C2Cl3F3/c3-1(4,5)2(6,7)8 |
| **InchiKey:** | BOSAWIQFTJIYIS-UHFFFAOYSA-N |
| **Formula:** | C2Cl3F3 |
| **SMILES:** | FC(F)(F)C(Cl)(Cl)Cl |
| **Mol. weight [g/mol]:** | 187.38 |
| **CAS:** | 354-58-5 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -648.58 | kJ/mol | Joback Method |
| hf | -737.66 | kJ/mol | Joback Method |
| hfus | 7.94 | kJ/mol | Joback Method |
| hvap | 28.10 ± 0.10 | kJ/mol | NIST Webbook |
| hvap | 29.20 | kJ/mol | NIST Webbook |
| hvap | 28.32 | kJ/mol | NIST Webbook |
| ie | 11.80 | eV | NIST Webbook |
| ie | 11.78 ± 0.03 | eV | NIST Webbook |
| ie | 11.50 | eV | NIST Webbook |
| log10ws | -2.88 | | Crippen Method |
| logp | 2.919 | | Crippen Method |
| mcvol | 81.070 | ml/mol | McGowan Method |

| | | | |
|---|---|---|---|
| pc | 3819.82 | kPa | Joback Method |
| rinpol | 527.00 | | NIST Webbook |
| rinpol | 520.00 | | NIST Webbook |
| rinpol | 525.00 | | NIST Webbook |
| rinpol | 530.00 | | NIST Webbook |
| tb | 319.20 | K | NIST Webbook |
| tb | 318.80 | K | NIST Webbook |
| tb | 319.00 | K | NIST Webbook |
| tb | 319.15 | K | Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa |
| tb | 319.00 ± 3.00 | K | NIST Webbook |
| tc | 482.90 | K | NIST Webbook |
| tf | 287.52 ± 0.01 | K | NIST Webbook |
| tf | 287.00 ± 2.00 | K | NIST Webbook |
| tt | 287.52 ± 0.01 | K | NIST Webbook |
| vc | 0.327 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 137.83 | J/mol×K | 410.49 | Joback Method |
| cpg | 153.48 | J/mol×K | 533.87 | Joback Method |
| cpg | 150.28 | J/mol×K | 503.02 | Joback Method |
| cpg | 146.63 | J/mol×K | 472.18 | Joback Method |
| cpg | 142.49 | J/mol×K | 441.33 | Joback Method |
| cpg | 126.81 | J/mol×K | 348.80 | Joback Method |
| cpg | 132.62 | J/mol×K | 379.64 | Joback Method |
| cpl | 168.60 | J/mol×K | 298.16 | NIST Webbook |
| hvapt | 28.90 | kJ/mol | 308.00 | NIST Webbook |
| hvapt | 26.30 ± 0.10 | kJ/mol | 328.00 | NIST Webbook |
| hvapt | 27.20 ± 0.10 | kJ/mol | 313.00 | NIST Webbook |
| hvapt | 26.85 | kJ/mol | 319.20 | NIST Webbook |
| pvap | 101.30 | kPa | 319.15 | Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.48158e+01 |
| Coeff. B | -3.05174e+03 |
| Coeff. C | -1.95350e+01 |
| Temperature range (K), min. | 229.59 |
| Temperature range (K), max. | 341.35 |

# Sources

| | |
|---|---|
| **Vapor Liquid Equilibrium for the 1,1,1-Trifluorotrichloroethane + Sulfuryl Chloride System at 101.3 kPa:** | https://www.doi.org/10.1021/je400544h |
| **Solubility Differences of Halocarbon Isomers in Ionic Liquid [emim][Tf2N]:** | https://www.doi.org/10.1021/je700295e |
| **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=C354585&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/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **cpl:** | Liquid phase heat capacity |
| **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 |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **tt:** | Triple Point Temperature |
| **vc:** | Critical Volume |