

Ethane, 1,1,1,2-tetrachloro-2,2-difluoro-

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|-----------------------------|---|
| Other names: | 1,1,1,2-Tetrachloro-2,2-difluoroethane 1,1,1,2-Tetrachlorodifluoroethane 1,1-Difluoro-1,2,2,2-tetrachloroethane 1,1-Difluorotetrachloroethane 1,2,2,2-Tetrachloro-1,1-difluoroethane 2,2-DIFLUORO-1,1,1,2-TETRACHLOROETHANE 2,2-Difluorotetrachloroethane CFC 112a Ethane, 2,2-difluoro-1,1,1,2-tetrachloro- F 112a FREON BU Halocarbon 112a R 112a REFRIGERANT-112A Refrigerant 112a |
| Inchi: | InChI=1S/C2Cl4F2/c3-1(4,5)2(6,7)8 |
| InchiKey: | SLGOCMATMKJJCE-UHFFFAOYSA-N |
| Formula: | C2Cl4F2 |
| SMILES: | FC(F)(Cl)C(Cl)(Cl)Cl |
| Mol. weight [g/mol]: | 203.83 |
| CAS: | 76-11-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -465.70 | kJ/mol | Joback Method |
| hf | -557.29 | kJ/mol | Joback Method |
| hfus | 9.06 | kJ/mol | Joback Method |
| hvap | 33.36 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 3.188 | | Crippen Method |
| mcvol | 91.540 | ml/mol | McGowan Method |
| pc | 3857.88 | kPa | Joback Method |
| rinpol | 702.00 | | NIST Webbook |
| rinpol | 785.00 | | NIST Webbook |
| rinpol | 785.00 | | NIST Webbook |
| rinpol | 702.00 | | NIST Webbook |
| tb | 364.70 | K | NIST Webbook |

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|----|---------------|----------------------|---------------|
| tb | 364.60 | K | NIST Webbook |
| tc | 592.71 | K | Joback Method |
| tf | 314.20 ± 0.20 | K | NIST Webbook |
| vc | 0.357 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 138.37 | J/mol×K | 386.96 | Joback Method |
| cpg | 143.76 | J/mol×K | 421.25 | Joback Method |
| cpg | 148.47 | J/mol×K | 455.54 | Joback Method |
| cpg | 152.57 | J/mol×K | 489.84 | Joback Method |
| cpg | 156.09 | J/mol×K | 524.13 | Joback Method |
| cpg | 159.09 | J/mol×K | 558.42 | Joback Method |
| cpg | 161.61 | J/mol×K | 592.71 | Joback Method |
| hfust | 3.99 | kJ/mol | 314.20 | NIST Webbook |
| sfust | 12.70 | J/mol×K | 314.20 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.34757e+01 |
| Coeff. B | -2.54565e+03 |
| Coeff. C | -7.72440e+01 |
| Temperature range (K), min. | 270.27 |
| Temperature range (K), max. | 389.05 |

| Information | Value |
|-----------------------------|--|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$ |
| Coeff. A | 9.41240e+01 |
| Coeff. B | -6.96532e+03 |
| Coeff. C | -1.22355e+01 |
| Coeff. D | 1.27074e-05 |
| Temperature range (K), min. | 262.15 |

Sources

| | |
|---|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C76119&Units=SI |
| 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=1542 |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| KDB: | https://www.thermo.com/files/research/kdb/mol/mol1542.mol |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{fust}: | Enthalpy of fusion at a given temperature |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pv_{ap}: | Vapor pressure |
| ri_{npol}: | Non-polar retention indices |
| sf_{ust}: | Entropy of fusion at a given temperature |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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