# 1,1,1-Trifluoro-2-propanol

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|---|---|
| **Other names:** | 1,1,1-Trifluoroisopropanol |
| | 1,1,1-Trifluoropropan-2-ol |
| | 1,1,1-Trifluoropropanol-2 |
| | 1-Methyl-2,2,2-trifluoroethanol |
| | 2-Propanol, 1,1,1-trifluoro- |
| **Inchi:** | InChI=1S/C3H5F3O/c1-2(7)3(4,5)6/h2,7H,1H3 |
| **InchiKey:** | GILIYJDBJZWGBG-UHFFFAOYSA-N |
| **Formula:** | C3H5F3O |
| **SMILES:** | CC(O)C(F)(F)F |
| **Mol. weight [g/mol]:** | 114.07 |
| **CAS:** | 374-01-6 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -746.47 | kJ/mol | Joback Method |
| hf | -859.84 | kJ/mol | Joback Method |
| hfus | 5.92 | kJ/mol | Joback Method |
| hvap | 44.80 | kJ/mol | NIST Webbook |
| hvap | 44.79 | kJ/mol | NIST Webbook |
| log10ws | 0.30 | | Aqueous Solubility Prediction Method |
| logp | 0.930 | | Crippen Method |
| mcvol | 64.310 | ml/mol | McGowan Method |
| pc | 4316.89 | kPa | Joback Method |
| tb | 354.36 | K | Joback Method |
| tc | 504.33 | K | Joback Method |
| tf | 173.58 | K | Joback Method |
| vc | 0.260 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 155.37 | J/mol×K | 479.34 | Joback Method |
| cpg | 127.15 | J/mol×K | 354.36 | Joback Method |

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|---|---|---|---|---|
| cpg | 133.41 | J/mol×K | 379.36 | Joback Method |
| cpg | 139.35 | J/mol×K | 404.35 | Joback Method |
| cpg | 144.98 | J/mol×K | 429.35 | Joback Method |
| cpg | 150.32 | J/mol×K | 454.34 | Joback Method |
| cpg | 160.15 | J/mol×K | 504.33 | Joback Method |
| hvapt | 44.20 | kJ/mol | 312.50 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.58046e+01 |
| Coeff. B | -3.07220e+03 |
| Coeff. C | -7.35100e+01 |
| Temperature range (K), min. | 271.50 |
| Temperature range (K), max. | 366.29 |

# Sources

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**Aqueous Solubility Prediction Method:** http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C374016&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

# Legend

**cpg:** Ideal gas 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

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|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |