# 1,1,1-trifluorodecane

**Other names:** Decane, 1,1,1-trifluoro
**Inchi:** InChI=1S/C10H19F3/c1-2-3-4-5-6-7-8-9-10(11,12)13/h2-9H2,1H3
**InchiKey:** IGGXVAUUTYVHBN-UHFFFAOYSA-N
**Formula:** C10H19F3
**SMILES:** CCCCCCCCCC(F)(F)F
**Mol. weight [g/mol]:** 196.25
**CAS:** 26288-16-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.5405 | | Cheméo Relay (1.0) |
| gf | -548.27 | kJ/mol | Joback Method |
| hf | -899.29 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 23.48 | kJ/mol | Joback Method |
| hvap | 45.30 | kJ/mol | Cheméo Relay (1.0) |
| ie | 10.81 | eV | Cheméo Relay (1.0) |
| log10ws | -5.24 | | Cheméo Relay (1.0) |
| logp | 4.689 | | Crippen Method |
| mcvol | 157.070 | ml/mol | McGowan Method |
| pc | 1900.26 | kPa | Joback Method |
| tb | 424.69 | K | Cheméo Relay (1.0) |
| tc | 559.29 | K | Cheméo Relay (1.0) |
| tf | 209.09 | K | Cheméo Relay (1.0) |
| vc | 0.610 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 341.37 | J/mol×K | 422.78 | Joback Method |
| cpg | 355.77 | J/mol×K | 447.54 | Joback Method |
| cpg | 369.59 | J/mol×K | 472.30 | Joback Method |
| cpg | 382.84 | J/mol×K | 497.07 | Joback Method |
| cpg | 395.54 | J/mol×K | 521.83 | Joback Method |
| cpg | 407.70 | J/mol×K | 546.59 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 419.36 | J/mol×K | 571.35 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.29907e+01 |
| Coeff. B | -3.38340e+03 |
| Coeff. C | -6.06000e+01 |
| Temperature range (K), min. | 326.94 |
| Temperature range (K), max. | 501.19 |

# Sources

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

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

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C26288164&Units=SI

# Legend

**af:** Acentric Factor

**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

**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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |