# 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propen

**Other names:** 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)propene
1,1-Difluoro-2,2-bis(trifluoromethyl)ethene
1-Propene, 1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-
Isobutene, octafluoro-
Octafluoro-sec-butene
Octafluoroisobutene
Octafluoroisobutylene
PFIB
Perfluorisobutylene
Perfluoro-2-(trifluoromethyl)propene
Perfluoro-2-methylpropene
Perfluoroisobutene
Perfluoroisobutylene
Propene, 1,1,3,3,3-pentafluoro-2-(trifluoromethyl)-
Propene, pentafluoro-2-(trifluoromethyl)-

**Inchi:** InChI=1S/C4F8/c5-2(6)1(3(7,8)9)4(10,11)12

**InchiKey:** DAFIBNSJXIGBQB-UHFFFAOYSA-N

**Formula:** C4F8

**SMILES:** FC(F)=C(C(F)(F)F)C(F)(F)F

**Mol. weight [g/mol]:** 200.03

**CAS:** 382-21-8

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1506.88 | kJ/mol | Joback Method |
| hf | -1614.63 | kJ/mol | Joback Method |
| hfus | 13.51 | kJ/mol | Joback Method |
| hvap | 15.49 | kJ/mol | Joback Method |
| log10ws | -3.37 | | Crippen Method |
| logp | 3.262 | | Crippen Method |
| mcvol | 77.080 | ml/mol | McGowan Method |
| pc | 2884.30 | kPa | Joback Method |
| tb | 282.54 | K | Joback Method |
| tc | 409.82 | K | Joback Method |
| tf | 111.40 | K | Joback Method |
| vc | 0.363 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 143.06 | J/mol×K | 282.54 | Joback Method |
| cpg | 151.05 | J/mol×K | 303.75 | Joback Method |
| cpg | 158.59 | J/mol×K | 324.97 | Joback Method |
| cpg | 165.70 | J/mol×K | 346.18 | Joback Method |
| cpg | 172.38 | J/mol×K | 367.39 | Joback Method |
| cpg | 178.65 | J/mol×K | 388.60 | Joback Method |
| cpg | 184.53 | J/mol×K | 409.82 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.63442e+01 |
| Coeff. B | -2.94460e+03 |
| Coeff. C | -1.90320e+01 |
| Temperature range (K), min. | 202.42 |
| Temperature range (K), max. | 299.15 |

# Sources

**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

**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=C382218&Units=SI

# 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 |
| **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 |