# 1,1,1,3,3,3-Hexafluoro-2-(trifluoromethyl)-2-propan

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|---|---|
| **Other names:** | Perfluoro-tert-butanol |
| | (CF3)3COH |
| | Perfluoro-t-butanol |
| | 2-Propanol, 1,1,1,3,3,3-hexafluoro-2-(trifluoromethyl)- |
| | Nonafluor-terc.butanol |
| | Nonafluoro-tert-butanol |
| | Ethanol, 2,2,2-trifluoro-1,1-bis(trifluoromethyl)- |
| | perfluoro-tert-butyl alcohol |
| **Inchi:** | InChI=1S/C4HF9O/c5-2(6,7)1(14,3(8,9)10)4(11,12)13/h14H |
| **InchiKey:** | XZNOAVNRSFURIR-UHFFFAOYSA-N |
| **Formula:** | C4HF9O |
| **SMILES:** | OC(C(F)(F)F)(C(F)(F)F)C(F)(F)F |
| **Mol. weight [g/mol]:** | 236.04 |
| **CAS:** | 2378-02-1 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 676.80 | kJ/mol | NIST Webbook |
| basg | 646.70 | kJ/mol | NIST Webbook |
| gf | -1895.95 | kJ/mol | Joback Method |
| hf | -2078.11 | kJ/mol | Joback Method |
| hfus | 8.27 | kJ/mol | Joback Method |
| hvap | 28.64 | kJ/mol | Joback Method |
| ie | 12.25 | eV | NIST Webbook |
| log10ws | -2.86 | | Crippen Method |
| logp | 2.404 | | Crippen Method |
| mcvol | 89.020 | ml/mol | McGowan Method |
| pc | 2956.90 | kPa | Joback Method |
| tb | 363.61 | K | Joback Method |
| tc | 493.06 | K | Joback Method |
| tf | 210.65 | K | Joback Method |
| vc | 0.397 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 213.43 | J/mol×K | 363.61 | Joback Method |
| cpg | 221.97 | J/mol×K | 385.19 | Joback Method |
| cpg | 229.94 | J/mol×K | 406.76 | Joback Method |
| cpg | 237.35 | J/mol×K | 428.34 | Joback Method |
| cpg | 244.25 | J/mol×K | 449.91 | Joback Method |
| cpg | 250.63 | J/mol×K | 471.49 | Joback Method |
| cpg | 256.54 | J/mol×K | 493.06 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C2378021&Units=SI
**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

# Legend

**affp:** Proton affinity
**basg:** Gas basicity
**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
**tb:** Normal Boiling Point Temperature
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point

**vc:** Critical Volume