# 2,2,3,3,3-Pentafluoro-1-propanol

| | |
|---|---|
| **Other names:** | 1,1-Dihydroperfluoropropanol |
| | 1,1H-perfluoropropanol |
| | 1-Propanol, 2,2,3,3,3-pentafluoro- |
| | 1H,1H-Pentafluoropropanol |
| | 1H,1H-Pentafluoropropanol-1 |
| | 2,2,3,3,3-Pentafluoropropanol |
| | C2F5CH2OH |
| | NSC 66413 |
| **Inchi:** | InChI=1S/C3H3F5O/c4-2(5,1-9)3(6,7)8/h9H,1H2 |
| **InchiKey:** | PSQZJKGXDGNDFP-UHFFFAOYSA-N |
| **Formula:** | C3H3F5O |
| **SMILES:** | OCC(F)(F)C(F)(F)F |
| **Mol. weight [g/mol]:** | 150.05 |
| **CAS:** | 422-05-9 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chl | -1149.70 ± 2.80 | kJ/mol | NIST Webbook |
| gf | -1130.81 | kJ/mol | Joback Method |
| hf | -1255.53 | kJ/mol | Joback Method |
| hfl | -1354.70 ± 2.90 | kJ/mol | NIST Webbook |
| hfus | 8.19 | kJ/mol | Joback Method |
| hvap | 44.40 | kJ/mol | NIST Webbook |
| hvap | 44.38 | kJ/mol | NIST Webbook |
| hvap | 41.30 | kJ/mol | NIST Webbook |
| ie | 11.68 | eV | NIST Webbook |
| ie | 11.20 | eV | NIST Webbook |
| log10ws | -1.32 | | Crippen Method |
| logp | 1.176 | | Crippen Method |
| mcvol | 67.850 | ml/mol | McGowan Method |
| pc | 3901.37 | kPa | Joback Method |
| tb | 353.70 | K | NIST Webbook |
| tb | 355.00 | K | NIST Webbook |
| tc | 490.34 | K | Joback Method |
| tf | 192.18 | K | Joback Method |
| vc | 0.290 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 144.58 | J/mol×K | 350.11 | Joback Method |
| cpg | 151.21 | J/mol×K | 373.48 | Joback Method |
| cpg | 157.44 | J/mol×K | 396.85 | Joback Method |
| cpg | 163.28 | J/mol×K | 420.22 | Joback Method |
| cpg | 168.76 | J/mol×K | 443.59 | Joback Method |
| cpg | 173.89 | J/mol×K | 466.96 | Joback Method |
| cpg | 178.69 | J/mol×K | 490.34 | Joback Method |
| hvapt | 45.10 | kJ/mol | 313.01 | Vapor pressure and liquid density of fluorinated alcohols: experimental, simulation and GC-SAFT-VR predictions |
| hvapt | 47.00 | kJ/mol | 285.00 | NIST Webbook |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 353.20 | K | 99.70 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.35801e+01 |
| Coeff. B | -2.22287e+03 |
| Coeff. C | -1.06110e+02 |
| Temperature range (K), min. | 273.00 |
| Temperature range (K), max. | 374.94 |

# Sources

| | |
|---|---|
| **Vapor pressure and liquid density of fluorinated alcohols: experimental, simulation and GC-SAFT-VR predictions:** | https://www.doi.org/10.1016/j.fluid.2016.06.011 |
| **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=C422059&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 |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Fluorinated surfactants in solution: Diffusion coefficients of fluorinated alcohols in water:** | https://www.doi.org/10.1016/j.fluid.2015.06.006 |

# Legend

| | |
|---|---|
| **chl:** | Standard liquid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfl:** | Liquid phase 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 |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

Latest version available from:
https://www.chemeo.com/cid/51-873-6/2-2-3-3-3-Pentafluoro-1-propanol.pdf
Generated by Cheméo on 2024-04-20 11:06:35.889244558 +0000 UTC m=+15900444.809821873.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.