

# 2-Propanol, 1,1,1,3,3,3-hexafluoro-

**Other names:** 1,1,1,3,3,3-Hexafluoro-2-hydroxypropane  
1,1,1,3,3,3-Hexafluoro-2-propanol  
1,1,1,3,3,3-Hexafluoroisopropanol  
1,1,1,3,3,3-Hexafluoroisopropyl alcohol  
1,1,1,3,3,3-Hexafluoropropan-2-ol  
1,1,1,3,3,3-Hexafluoropropanol  
2,2,2-Trifluoro-1-(trifluoromethyl)ethanol  
2H-Hexafluoroisopropanol  
Bis(trifluoromethyl)methanol  
CF3CH(OH)CF3  
Ethanol, 2,2,2-trifluoro-1-(trifluoromethyl)-  
HFIP  
Hexafluoro-2-propanol  
Hexafluoroisopropanol  
Hexafluoroisopropyl alcohol  
NSC 96336

**Inchi:** InChI=1S/C3H2F6O/c4-2(5,6)1(10)3(7,8)9/h1,10H

**InchiKey:** BYEAHWXPCBROCE-UHFFFAOYSA-N

**Formula:** C3H2F6O

**SMILES:** OC(C(F)(F)F)C(F)(F)F

**Mol. weight [g/mol]:** 168.04

**CAS:** 920-66-1

## Physical Properties

Property code	Value	Unit	Source
affp	686.60	kJ/mol	NIST Webbook
basg	656.20	kJ/mol	NIST Webbook
gf	-1328.06	kJ/mol	Joback Method
hf	-1456.92	kJ/mol	Joback Method
hfus	7.74	kJ/mol	Joback Method
hvap	41.60	kJ/mol	NIST Webbook
hvap	41.58	kJ/mol	NIST Webbook
ie	11.94	eV	NIST Webbook
ie	12.23	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.472		Crippen Method
mcvol	69.620	ml/mol	McGowan Method

pc	3727.11	kPa	Joback Method
tb	332.20	K	NIST Webbook
tb	331.00	K	NIST Webbook
tc	485.00	K	Joback Method
tf	177.77	K	Joback Method
vc	0.302	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.81	J/mol×K	462.32	Joback Method
cpg	152.66	J/mol×K	348.94	Joback Method
cpg	159.24	J/mol×K	371.62	Joback Method
cpg	165.43	J/mol×K	394.29	Joback Method
cpg	171.24	J/mol×K	416.97	Joback Method
cpg	176.70	J/mol×K	439.65	Joback Method
cpg	186.58	J/mol×K	485.00	Joback Method
hvapt	40.20	kJ/mol	312.00	NIST Webbook
hvapt	47.30	kJ/mol	284.50	NIST Webbook
rhol	1604.84	kg/m3	298.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vap}}) = A + B/(T + C)$
Coeff. A	1.72410e+01
Coeff. B	-3.76991e+03
Coeff. C	-3.34880e+01
Temperature range (K), min.	255.86
Temperature range (K), max.	349.50

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C920661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C920661&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorobutanesulfonic Acid + Water at 298.15 K: Part II. Solubilities of noble Gases</b>	<a href="https://www.doi.org/10.1021/je500455u">https://www.doi.org/10.1021/je500455u</a>
<b>1,1,1,3,3,3-hexafluoropropan-2-ol at 298.15 K and 101.33 kPa: Solubility of gases in fluororganic alcohols. Part III. Solubilities of several non-polar gases in water + 1,1,1,3,3,3-hexafluoropropan-2-ol at 298.15 K and 101.33 kPa:</b>	<a href="https://www.doi.org/10.1016/j.jct.2011.11.019">https://www.doi.org/10.1016/j.jct.2011.11.019</a>
	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
	<a href="https://www.doi.org/10.1016/j.jct.2018.12.027">https://www.doi.org/10.1016/j.jct.2018.12.027</a>

## Legend

<b>affp:</b>	Proton affinity
<b>basg:</b>	Gas basicity
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>rhol:</b>	Liquid Density
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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