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-Hexafluoropropan-2-ol
	1,1,1,3,3,3-Hexafluoropropanol
	1,1,1,3,3,3-hexafluoro-2-propanol
	1,1,1,3,3,3-hexafluoroisopropanol
	1,1,1,3,3,3-hexafluoroisopropyl alcohol
	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
hfus	7.74	kJ/mol	Joback Method
hvap	41.58	kJ/mol	NIST Webbook
hvap	41.60	kJ/mol	NIST Webbook
ie	11.94	eV	NIST Webbook
ie	12.23	eV	NIST Webbook
log10ws	-0.98		Cheméo Relay (1.0)
logp	1.472		Crippen Method
mcvol	69.620	ml/mol	McGowan Method
tb	331.00	K	NIST Webbook
tb	332.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	181.81	J/mol×K	462.32	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(Pvp) = 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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of gases in fluoroorganic 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:	https://www.doi.org/10.1016/j.jct.2018.12.027
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Solubility of gases in fluoroorganic alcohols. Part II. Solubilities of noble gases in (water + 1,1,1,3,3,3-hexafluoropropan-2-ol) at 298.15 K and 101.33 kPa:	https://www.doi.org/10.1016/j.jct.2011.11.019
Liquid–Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorohexane + Water or Methanol at 298.15 K:	https://www.doi.org/10.1021/je500455u
NIST Chemistry WebBook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C920661&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature