2,2,3,3-Tetrafluoro-1-propanol

Other names:	1,1,2,2-tetrafluoro-3-hydroxypropane
	1,1,3-Trihydroperfluoro-1-propanol
	1,1,3H-perfluoropropanol
	1-Propanol, 2,2,3,3-tetrafluoro-
	1-hydroxy-2,2,3,3-tetrafluoropropane
	1H,1H,3H-Tetrafluoro-1-propanol
	2,2,3,3-Tetrafluoro-propanol-1
	2,2,3,3-Tetrafluoropropanol
	2,2,3,3-Tetrafluoropropyl alcohol
	2,2,3,3-tetrafluoropropan-1-ol
	2,2,3,3-tetrafluoropropanol-1
Inchi:	InChI=1S/C3H4F4O/c4-2(5)3(6,7)1-8/h2,8H,1H2
InchiKey:	NBUKAOOFKZFCGD-UHFFFAOYSA-N
Formula:	C3H4F4O
SMILES:	OCC(F)(F)C(F)F
Mol. weight [g/mol]:	132.06
CAS:	76-37-9

Physical Properties

Property code	Value	Unit	Source
chl	-1353.40 ± 0.67	kJ/mol	NIST Webbook
gf	-941.28	kJ/mol	Joback Method
hf	-1055.95	kJ/mol	Joback Method
hfl	-1114.90 ± 0.79	kJ/mol	NIST Webbook
hfus	9.00	kJ/mol	Joback Method
hvap	53.58	kJ/mol	NIST Webbook
hvap	53.60	kJ/mol	NIST Webbook
ie	11.58	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	0.879		Crippen Method
mcvol	66.080	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	640.00		NIST Webbook
rinpol	636.00		NIST Webbook
rinpol	651.00		NIST Webbook
tb	382.70	K	NIST Webbook

tb	382.15	K	Separation of azeotrope (2,2,3,3-tetrafluoro-1-propanol + water): Isobaric vapour-liquid phase equilibrium measurements and azeotropic distillation
tb	381.95	K	Separation of azeotropic mixture (2, 2, 3, 3-Tetrafluoro-1-propanol + water) by extractive distillation: Entrainers selection and vapour-liquid equilibrium measurements
tb	382.50 ± 0.50	K	NIST Webbook
tc	495.89	K	Joback Method
tf	174.17	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.15	J/mol×K	495.89	Joback Method
cpg	135.42	J/mol×K	353.63	Joback Method
cpg	162.54	J/mol×K	472.18	Joback Method
cpg	157.67	J/mol×K	448.47	Joback Method
cpg	152.54	J/mol×K	424.76	Joback Method
cpg	147.12	J/mol×K	401.05	Joback Method
cpg	141.42	J/mol×K	377.34	Joback Method
hvapt	50.30	kJ/mol	315.50	NIST Webbook
hvapt	47.90	kJ/mol	341.50	NIST Webbook
pvap	101.30	kPa	382.15	Separation of azeotrope (2,2,3,3-tetrafluoro-1-propanol + water): Isobaric vapour-liquid phase equilibrium measurements and azeotropic distillation
pvap	101.30	kPa	381.95	Separation of azeotropic mixture (2, 2, 3, 3-Tetrafluoro-1-propanol + water) by extractive distillation: Entrainers selection and vapour-liquid equilibrium measurements

pvap	53.30	kPa	365.01	Isobaric Vapor Liquid Equilibrium for Binary Systems of 2,2,3,3-Tetrafluoro-1-propanol + 2,2,3,3,4,4,5,5-Octafluoro-1-pentanol at 53.3, 66.7, 80.0 kPa
pvap	66.70	kPa	370.79	Isobaric Vapor Liquid Equilibrium for Binary Systems of 2,2,3,3-Tetrafluoro-1-propanol + 2,2,3,3,4,4,5,5-Octafluoro-1-pentanol at 53.3, 66.7, 80.0 kPa
pvap	80.00	kPa	375.66	Isobaric Vapor Liquid Equilibrium for Binary Systems of 2,2,3,3-Tetrafluoro-1-propanol + 2,2,3,3,4,4,5,5-Octafluoro-1-pentanol at 53.3, 66.7, 80.0 kPa
rfi	1.31960		303.15	Liquid-liquid equilibrium for ternary systems of ethyl acetate/isopropyl acetate + 2,2,3,3-tetrafluoro-1-propanol + water at 298.15, 318.15 K
rhol	1482.80	kg/m3	301.55	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1434.00	kg/m3	327.05	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1427.40	kg/m3	330.65	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols

rhol	1416.80	kg/m3	334.35	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1409.00	kg/m3	338.25	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1401.00	kg/m3	342.25	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1441.80	kg/m3	323.25	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1493.20	kg/m3	293.15	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1454.20	kg/m3	316.15	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1460.20	kg/m3	312.65	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1468.60	kg/m3	309.05	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols
rhol	1474.20	kg/m3	306.15	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols

rhol	1447.60	kg/m3	319.35	Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48751e+01
Coeff. B	-3.02459e+03
Coeff. C	-8.77620e+01
Temperature range (K), min.	295.10
Temperature range (K), max.	404.02

Sources

Separation of azeotropic mixture (2, 2, 3, 3-Tetrafluoro-1-propanol + water) by extractive distillation: Entrainers selection and vapor-liquid equilibrium measurements:	https://www.doi.org/10.1016/j.jct.2019.06.026
Measurements and correlations of density, viscosity, and vapour-liquid equilibrium for fluoro alcohols:	https://www.doi.org/10.1016/j.jct.2016.07.011
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibrium for ternary systems of water + 2,2,3,3-tetrafluoro-1-propanol + isopropyl ether at 298.2, 308.2 K:	https://www.doi.org/10.1016/j.jct.2018.04.006
Liquid-liquid equilibrium for ternary systems of ethyl acetate/isopropyl acetate/tert-butyl methyl ether + water at 298.15, 318.15 K:	https://www.doi.org/10.1016/j.jct.2016.12.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Modified UNIFAC (Dortmund) Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isobaric Vapor Liquid Equilibrium for Binary Systems of 2,2,3,3-Tetrafluoro-1-propanol + 2,2,3,3,4,4,5,5-Octafluoro-1-pentanol at 333, 66.7, 80.0 kPa:	https://www.doi.org/10.1021/acs.jced.6b00429
Liquid-Liquid Equilibrium for Ternary Systems of Water + 2,2,3,3-Tetrafluoro-1-propanol + Anisole/1-Octanol at 298.2, 308.2, and 318.2 K:	https://www.doi.org/10.1021/acs.jced.8b00393
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Separation of azeotrope (2,2,3,3-tetrafluoro-1-propanol + water): Isobaric vapour-liquid phase equilibrium measurements and azeotropic distillation:	https://www.doi.org/10.1016/j.jct.2017.07.019

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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume