Perfluorooctane

Other names:	OCTADECAFLUOROOCTANE
	Octane, octadecafluoro-
	Perfluorooctanes
	n-Perfluorooctane
Inchi:	InChI=1S/C8F18/c9-1(10,3(13,14)5(17,18)7(21,22)23)2(11,12)4(15,16)6(19,20)8(24,25)2
InchiKey:	YVBBRRALBYAZBM-UHFFFAOYSA-N
Formula:	C8F18
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	438.06
CAS:	307-34-6

Physical Properties

Property code	Value	Unit	Source
gf	-3467.38	kJ/mol	Joback Method
hf	-3808.43	kJ/mol	Joback Method
hfus	12.60	kJ/mol	Joback Method
hvap	41.16	kJ/mol	NIST Webbook
hvap	41.10 ± 0.10	kJ/mol	NIST Webbook
hvap	41.20 ± 0.80	kJ/mol	NIST Webbook
hvap	39.90	kJ/mol	NIST Webbook
log10ws	-6.38		Crippen Method
logp	5.923		Crippen Method
mcvol	155.440	ml/mol	McGowan Method
pc	1660.00	kPa	KDB
rinpol	341.00		NIST Webbook
rinpol	341.00		NIST Webbook
tb	379.00	K	NIST Webbook
tb	379.00	K	KDB
tb	372.50 ± 0.50	K	NIST Webbook
tb	377.20	K	NIST Webbook
tc	502.00	K	KDB
tc	502.30 ± 0.50	K	NIST Webbook
tf	254.20 ± 0.50	K	NIST Webbook
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.73	J/mol×K	396.41	Joback Method
cpg	389.83	J/mol×K	361.11	Joback Method
cpg	403.16	J/mol×K	378.76	Joback Method
cpg	427.56	J/mol×K	414.06	Joback Method
cpg	438.69	J/mol×K	431.72	Joback Method
cpg	449.13	J/mol×K	449.37	Joback Method
cpg	375.72	J/mol×K	343.46	Joback Method
hfust	9.58	kJ/mol	254.20	NIST Webbook
hvapt	33.38	kJ/mol	379.00	NIST Webbook
hvapt	32.00	kJ/mol	470.00	NIST Webbook
hvapt	39.50	kJ/mol	344.50	NIST Webbook
kvisc	0.0000007	m2/s	298.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000006	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000006	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000007	m2/s	303.15	Viscosities of Liquid Fluorocompounds
pvap	10.10	kPa	318.42	Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation
pvap	42.35	kPa	352.86	High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K

pvap	6.10	kPa	308.45	Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation
pvap	19.23	kPa	332.87	High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K
pvap	12.80	kPa	323.48	Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation
pvap	29.02	kPa	342.87	High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K
pvap	24.30	kPa	338.43	Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation
pvap	7.77	kPa	312.78	High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K

pvap	12.42	kPa	322.79	High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K
pvap	16.00	kPa	328.48	Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation
rfi	1.26800		293.00	Binary Vapor-Liquid Equilibrium Data for Perfluorooctane with Light Gases (Oxygen, Nitrogen, and Methane)
rhol	1755.00	kg/m3	298.15	VLE measurements and modelling for the binary systems of (CF4 + C6F14) and (CF4 + C8F18)
rhol	1754.28	kg/m3	298.15	Liquid-liquid equilibrium data for binary perfluoroalkane (C6 and C8) + n-alkane systems
rhol	1760.93	kg/m3	292.84	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1722.71	kg/m3	307.51	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids

rhol	1755.00	kg/m3	298.15	Phase Equilibria for Perfluoroethane + (n-Perfluorohexane or n-Perfluorooctane) Binary Systems: Measurement and Modeling
rhol	1734.49	kg/m3	303.15	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1709.52	kg/m3	312.58	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1750.06	kg/m3	297.27	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
rhol	1770.70	kg/m3	289.03	Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids
speedsl	479.24	m/s	338.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	610.05	m/s	288.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT

speedsl	581.94	m/s	298.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	552.33	m/s	308.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	524.10	m/s	318.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	508.43	m/s	328.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	640.32	m/s	278.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
srf	0.02	N/m	288.05	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	293.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	298.35	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	303.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	308.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	318.75	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	323.85	Surface Tension of Liquid Fluorocompounds

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.37506e+01
Coeff. B	-7.19362e+03
Coeff. C	-8.56563e+00
Coeff. D	5.06612e-06
Temperature range (K), min.	308.15
Temperature range (K), max.	495.15

Sources

VLE measurements and modelling for the binary systems of (CF4 + C6F14) and (CF4 + C8F18):	https://www.doi.org/10.1016/j.fluid.2018.12.005
Perfluoroalkanes and perfluoroalkylalkane surfactants in solution: Partial molar volumes in n-octane and PHCT-SAFT-VR:	https://www.doi.org/10.1016/j.fluid.2011.02.020
Liquid-liquid equilibrium of (1H,1H,2H-perfluorohexan-1-ol + n-octane or n-perfluorooctane) binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.10.025
Isothermal vapor-liquid equilibrium of R170 + n-perfluorooctane at 308 - 338 K: Measurement, equation of state modelling, and molecular simulation:	https://www.doi.org/10.1016/j.fluid.2013.01.017
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1642.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Low pressure solubility and thermodynamics of solvation of oxygen, carbon dioxide, and carbon monoxide in fluorinated liquids:	https://www.doi.org/10.1016/j.jct.2006.11.012
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
Phase Separation in Binary Mixtures Containing Linear Perfluoroalkanes:	https://www.doi.org/10.1021/je049620w
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
High-pressure phase equilibria data for mixtures involving ethene and perfluoro-n-octane from 293 to 353 K:	https://www.doi.org/10.1016/j.fluid.2015.07.054
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Binary Vapor-Liquid Equilibrium Data for Perfluorooctane with Light Gases (Oxygen, Nitrogen, and Methane):	https://www.doi.org/10.1021/acs.jced.7b00657
Liquid-liquid equilibrium of (perfluoroalkane + alkane) binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.02.003
Liquid-liquid equilibrium data for binary perfluoroalkane (C6 and C8) + n-alkane systems:	https://www.doi.org/10.1016/j.fluid.2010.05.018
(Liquid + liquid) equilibria of perfluorocarbons with fluorinated ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.04.019
Phase Equilibria for Perfluoroethane + (n-Perfluorohexane or n-Perfluorooctane) Binary Systems: Measurement and Modeling:	https://www.doi.org/10.1021/acs.jced.6b00409
Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT:	https://www.doi.org/10.1016/j.fluid.2010.01.027
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C307346&Units=SI
Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies:	https://www.doi.org/10.1016/j.jct.2007.04.002
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1642
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
kvisc:	Kinematic viscosity
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
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume