Hexane, tetradecafluoro-

Other names:	AF 0150
	Fluorinert FC72
	Flutec PP1
	Hexane, 1,1,1,2,2,3,3,4,4,5,5,6,6,6-tetradecafluoro-
	PERFLUORO-N-HEXANE
	PERFLUOROHEXANE
	PP 1 (Fluorocarbon)
	Perflexane
	Perfluoro-compound FC-72
	TETRADECAFLUOROHEXANE
	flutec PP 1
	n-Perfluorohexane
	n-Tetradecafluorohexane
Inchi:	InChI=1S/C6F14/c7-1(8,3(11,12)5(15,16)17)2(9,10)4(13,14)6(18,19)20
InchiKey:	ZJIJAJXFLBMLCK-UHFFFAOYSA-N
Formula:	C6F14
SMILES:	FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	338.04
CAS:	355-42-0

Physical Properties

Property code	Value	Unit	Source
af	0.5140		KDB
gf	-2710.66	kJ/mol	Joback Method
hf	-2965.21	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	31.40	kJ/mol	NIST Webbook
hvap	32.40	kJ/mol	NIST Webbook
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
log10ws	-4.91		Crippen Method
logp	4.652		Crippen Method
mcvol	120.180	ml/mol	McGowan Method
pc	1868.13 ± 20.00	kPa	NIST Webbook
pc	1868.10 ± 3.44	kPa	NIST Webbook
pc	1905.00	kPa	NIST Webbook
pc	1868.00	kPa	KDB
rhoc	557.77 ± 3.04	kg/m3	NIST Webbook

rhoc	557.77 ± 5.58	kg/m3	NIST Webbook
tb	330.30	K	NIST Webbook
tb	332.50 ± 0.50	K	NIST Webbook
tb	332.20	K	NIST Webbook
tb	329.80	K	KDB
tc	448.77 ± 0.20	K	NIST Webbook
tc	448.77 ± 1.30	K	NIST Webbook
tc	448.77	K	KDB
tc	449.00	K	NIST Webbook
tc	447.65 ± 0.50	K	NIST Webbook
tc	451.70 ± 0.50	K	NIST Webbook
tf	182.50 ± 0.50	K	NIST Webbook
tf	186.00	K	KDB
tf	187.10 ± 0.10	K	NIST Webbook
tf	186.89 ± 0.06	K	NIST Webbook
tf	185.00 ± 1.00	K	NIST Webbook
tt	185.00 ± 2.00	K	NIST Webbook
tt	187.45 ± 0.30	K	NIST Webbook
vc	0.606	m3/kmol	KDB
zc	0.3033810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.57	J/mol×K	399.58	Joback Method
cpg	263.70	J/mol×K	307.08	Joback Method
cpg	288.03	J/mol×K	344.08	Joback Method
cpg	299.18	J/mol×K	362.58	Joback Method
cpg	309.69	J/mol×K	381.08	Joback Method
cpg	276.21	J/mol×K	325.58	Joback Method
cpg	328.86	J/mol×K	418.08	Joback Method
cpl	240.20	J/mol×K	273.00	NIST Webbook
cpl	248.00	J/mol×K	273.00	NIST Webbook
hfust	6.84	kJ/mol	185.00	NIST Webbook
hvapt	34.40	kJ/mol	297.50	NIST Webbook
hvapt	31.50	kJ/mol	316.50	NIST Webbook
hvapt	33.40	kJ/mol	441.00	NIST Webbook
kvisc	0.0000004	m2/s	313.15	Viscosities of Liquid Fluorocompounds

kvisc	0.0000004	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000004	m2/s	303.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000003	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000004	m2/s	298.15	Viscosities of Liquid Fluorocompounds
pvap	78.91	kPa	323.13	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	44.38	kPa	307.97	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	111.39	kPa	333.10	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	18.78	kPa	288.31	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	23.58	kPa	293.22	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	29.28	kPa	298.09	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	36.19	kPa	302.98	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	94.08	kPa	328.11	Densities and Vapor Pressures of Highly Fluorinated Compounds
pvap	54.56	kPa	313.17	Densities and Vapor Pressures of Highly Fluorinated Compounds

pvap	65.86	kPa	318.15	Densities and Vapor Pressures of Highly Fluorinated Compounds
rhol	1728.30	kg/m3	283.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1638.60	kg/m3	313.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1590.50	kg/m3	328.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1670.07	kg/m3	298.15	Liquid-liquid equilibrium data for binary perfluoroalkane (C6 and C8) + n-alkane systems
rhol	1701.00	kg/m3	298.15	VLE measurements and modelling for the binary systems of (CF4 + C6F14) and (CF4 + C8F18)
rhol	1667.00	kg/m3	298.15	Phase Equilibria for Perfluoroethane + (n-Perfluorohexane or n-Perfluorooctane) Binary Systems: Measurement and Modeling

rhol	1654.10	kg/m3	308.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1669.40	kg/m3	303.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1684.40	kg/m3	298.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1699.20	kg/m3	293.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1742.50	kg/m3	278.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1713.80	kg/m3	288.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K

rhol	1622.90	kg/m3	318.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1606.40	kg/m3	323.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
speedsl	510.70	m/s	298.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	540.31	m/s	288.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	571.89	m/s	278.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
srf	0.01	N/m	283.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	288.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	293.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	298.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	303.15	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	308.15	Surface Tension of Liquid Fluorocompounds

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49601e+01
Coeff. B	-3.09560e+03
Coeff. C	-3.28200e+01
Temperature range (K), min.	243.80
Temperature range (K), max.	353.65

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.25737e+02
Coeff. B	-7.95388e+03
Coeff. C	-1.70953e+01
Coeff. D	1.93783e-05
Temperature range (K), min.	270.00
Temperature range (K), max.	445.42

Datasets

Molar volume, m3/mol

Temperature, K - Liquid	Pressure, kPa - Liquid	Molar volume, m3/mol - Liquid
288.05	101.33	0.0002

Reference *https://www.doi.org/10.1016/j.jct.2007.04.002*

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

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1627
Liquid - Liquid Equilibria for the Ternary Systems of Per fl uorohexane + Methyl Nona- fl uorobutyl Ether + Toluene, + 1,4-Dioxane, or + Dimethylformamide at 298.15 K:	https://www.doi.org/10.1021/je301149f
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
Densities and Vapor Pressures of Highly Fluorinated Compounds:	https://www.doi.org/10.1021/je050056e
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Liquid Liquid Equilibria for the Ternary Systems of FC3283 + HFE7300 + Hexane, FC3283 + HFE7300 + Octane, and FC72 + HFE7100 + Acetonitrile or Ethyl Acetate at 298.15 K:	https://www.doi.org/10.1021/je500107y
High Pressure Vapor−Liquid Equilibria of Some Carbon Dioxide + Organic Liquid and Liquid−Liquid−Liquid Equilibria of Carbon Dioxide + Perfluoroalkane + Organic Liquid Systems at 298.15 K, 313.15 K:	https://www.doi.org/10.1021/je0498560
Liquid-liquid equilibria for perfluorohexane +CO2 + methanol, + toluene, and + acetone at 313K:	https://www.doi.org/10.1016/j.fluid.2005.12.041
Joback Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.10.025
Perfluoroalkanes and perfluoroalkylalkane surfactants in solution: Partial molar volumes in squalane and hetero-SAFT-VR modeling:	https://en.wikipedia.org/wiki/Joback_method
Liquid-Liquid Equilibria for the Ternary Systems of Perfluorohexane + Squalane + Hydrofluoroether + Tetrahydrofuran at 298.15 K or 273.15 K:	https://www.doi.org/10.1016/j.fluid.2011.02.020
KDB Amine:	https://www.doi.org/10.1021/je400227m
NIST Webbook:	https://www.cheric.org/files/research/kdb/mol/mol1627.mol
Thermodynamic study of (perfluoroalkane + alkane) mixtures: Excess and solvation enthalpies:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C355420&Units=SI
Properties of saturated fluoroarbons:	https://www.doi.org/10.1016/j.jct.2007.04.002
Experimental data and modeling using perturbed-chain SAFT:	https://www.doi.org/10.1016/j.fluid.2010.01.027
Viscosity of liquid systems involving hydrogenated and fluorinated substances: Liquid mixtures of (hexane + perfluorohexane):	https://www.doi.org/10.1016/j.fluid.2013.07.060
Phase Separation in Binary Mixtures Containing Linear Perfluoroalkanes:	https://www.doi.org/10.1021/je049620w
Phase Equilibria for Perfluoroethane + (n-Perfluorohexane or n-Perfluorooctane) Binary Systems: Measurement and Modeling:	https://www.doi.org/10.1021/acs.jced.6b00409
Liquid Liquid Coexistence Curve of n-Perfluorohexane + Hexane System:	https://www.doi.org/10.1007/s10765-007-0237-4
Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K:	https://www.doi.org/10.1021/je500455u
liquid-liquid equilibrium data for binary perfluoroalkane (C6 and C8) + n-alkane systems:	https://www.doi.org/10.1016/j.fluid.2010.05.018
New experimental VLE data for the binary mixture of carbon dioxide + perfluorohexane (CO2 + C6F14) from 273 K to 333 K:	https://www.doi.org/10.1016/j.fluid.2019.06.024
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-liquid equilibria containing fluorous solvents as environmentally benign solvent:	https://www.doi.org/10.1016/j.fluid.2012.12.037
Thermodynamic study of perfluorohexane + ether mixtures VLE, LLE, and HE:	https://www.doi.org/10.1016/j.fluid.2008.04.021
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Isothermal Vapor-Liquid Equilibrium (VLE) and Vapor- Liquid-Liquid Equilibrium (VLLE) Data for Two Binary Systems Containing Perfluorohexane with Carbon Monoxide or Hydrogen Sulphide at (298, 313 and 333) K:	https://www.doi.org/10.1021/acs.jced.5b00318

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rhoc:	Critical density
rhol:	Liquid Density
speedsl:	Speed of sound in fluid
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
volm:	Molar Volume
zc:	Critical Compressibility