Heptane, hexadecafluoro-

Other names:	HEXADECAFLUOROHEPTANE
	N-PERFLUOROHEPTANE
	PERFLUORO-N-HEPTANE
	Perfluoroheptane
Inchi:	InChI=1S/C7F16/c8-1(9,2(10,11)4(14,15)6(18,19)20)3(12,13)5(16,17)7(21,22)23
InchiKey:	LGUZHRODIJCVOC-UHFFFAOYSA-N
Formula:	C7F16
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)F
Mol. weight [g/mol]:	388.05
CAS:	335-57-9

Physical Properties

Property code	Value	Unit	Source
af	0.5560		KDB
chl	-1757.40 ± 0.88	kJ/mol	NIST Webbook
gf	-3089.00	kJ/mol	KDB
hf	-3387.00	kJ/mol	KDB
hfl	-3421.70 ± 3.60	kJ/mol	NIST Webbook
hfus	11.27	kJ/mol	Joback Method
hvap	35.90	kJ/mol	NIST Webbook
hvap	36.30 ± 0.30	kJ/mol	NIST Webbook
hvap	36.34	kJ/mol	NIST Webbook
log10ws	-5.65		Crippen Method
logp	5.288		Crippen Method
mcvol	137.810	ml/mol	McGowan Method
pc	1620.00	kPa	KDB
pc	1610.00 ± 13.78	kPa	NIST Webbook
pc	1620.00 ± 20.27	kPa	NIST Webbook
pc	1650.00 ± 150.00	kPa	NIST Webbook
pc	1620.00 ± 20.26	kPa	NIST Webbook
rhoc	582.07 ± 3.88	kg/m3	NIST Webbook
rhoc	588.67 ± 10.09	kg/m3	NIST Webbook
rinpol	263.00		NIST Webbook
rinpol	300.00		NIST Webbook
tb	354.00 ± 1.00	K	NIST Webbook
tb	355.66 ± 0.07	K	NIST Webbook
tb	355.00 ± 2.00	K	NIST Webbook

tb	355.60	K	NIST Webbook
tb	355.05 ± 0.50	K	NIST Webbook
tb	355.66	K	KDB
tb	354.65 ± 1.00	K	NIST Webbook
tb	355.45 ± 0.40	K	NIST Webbook
tc	477.80 ± 0.50	K	NIST Webbook
tc	474.70 ± 0.50	K	NIST Webbook
tc	474.80	K	KDB
tc	475.00 ± 2.00	K	NIST Webbook
tc	474.90 ± 0.50	K	NIST Webbook
tc	474.90 ± 0.60	K	NIST Webbook
tf	180.00 ± 0.20	K	NIST Webbook
tf	197.15 ± 1.50	K	NIST Webbook
tf	195.00	K	KDB
tt	221.87 ± 0.05	K	NIST Webbook
vc	0.664	m3/kmol	KDB
zc	0.2724810		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.17	J/mol×K	325.27	Joback Method
cpg	331.58	J/mol×K	343.32	Joback Method
cpg	344.25	J/mol×K	361.36	Joback Method
cpg	356.20	J/mol×K	379.41	Joback Method
cpg	367.46	J/mol×K	397.46	Joback Method
cpg	378.05	J/mol×K	415.51	Joback Method
cpg	387.99	J/mol×K	433.55	Joback Method
hfust	6.95	kJ/mol	221.90	NIST Webbook
hvapt	32.60	kJ/mol	418.50	NIST Webbook
hvapt	37.70	kJ/mol	325.00	NIST Webbook
hvapt	34.90	kJ/mol	324.00	NIST Webbook
kvisc	0.0000004	m2/s	318.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000004	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000005	m2/s	303.15	Viscosities of Liquid Fluorocompounds

kvisc	0.0000005	m2/s	298.15	Viscosities of Liquid Fluorocompounds
rhol	1733.00	kg/m3	293.00	KDB
rhol	1717.00	kg/m3	293.15	Binary vapour-liquid equilibrium data for C7 and C9 straight-chain perfluorocarbons with ethylene
speedsl	517.47	m/s	308.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	608.30	m/s	278.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	578.42	m/s	288.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	548.73	m/s	298.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	457.24	m/s	333.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	470.60	m/s	328.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT
speedsl	500.56	m/s	318.15	Properties of saturated fluorocarbons: Experimental data and modeling using perturbed-chain-SAFT

srf	0.01	N/m	293.25	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	289.05	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	318.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	313.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	308.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	303.45	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	298.25	Surface Tension of Liquid Fluorocompounds

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53638e+01
Coeff. B	-3.38459e+03
Coeff. C	-4.00210e+01
Temperature range (K), min.	264.52
Temperature range (K), max.	376.72

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.24433e+02
Coeff. B	-8.58006e+03
Coeff. C	-1.66191e+01
Coeff. D	1.52404e-05
Temperature range (K), min.	271.00
Temperature range (K), max.	470.92

Sources

Properties of saturated fluorocarbons:	https://www.doi.org/10.1016/j.fluid.2010.01.027
Experimental data and modeling using perturbed-chain SAFT:	https://www.doi.org/10.1016/j.fluid.2016.08.015
Binary vapour-liquid equilibrium data for C7 and C9 straight-chain perfluorocarbons with ethylene:	https://www.cheric.org/files/research/kdb/mol/mol1637.mol
KDB	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Phase Separation in Binary Mixtures Containing Linear Perfluoroalkanes:	https://www.doi.org/10.1021/je049620w
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C335579&Units=SI
Liquid liquid equilibrium of (1H,1H,7H-perfluoroheptan-1-ol + perfluoroalkane) binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.10.025
Thermodynamic study of (perfluoroalkane + alkane) mixtures:	https://www.doi.org/10.1016/j.jct.2007.04.002
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Excess and solvation enthalpies:	

Legend

af:	Acentric Factor
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
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
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
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility