Perfluoro(methylcyclohexane)

Other names:	(Trifluoromethyl)undecafluorocyclohexane (trifluoromethyl)undecaflurocyclohexane 1,1,2,2,3,3,4,4,5,5,6-Undecafluoro-6-(trifluoromethyl)cyclohexane Cyclohexane, 1,1,2,2,3,3,4,4,5,5,6-undecafluoro-6-(trifluoromethyl)- Cyclohexane, 1-trifluoromethyl-1,2,2,3,3,4,4,5,5,6,6-undecafluoro- Cyclohexane, undecafluoro(trifluoromethyl)- Flutec PP2 NSC 4779 Perfluoromethylcyclohexane Tetradecafluoromethylcyclohexane UNDECAFLUORO(TRIFLUOROMETHYL)-CYCLOHEXANE Undecafluoro(trifluoromethyl)cyclohexane cyclohexane, tetradecafluoromethyl-
Inchi:	InChI=1S/C7F14/c8-1(7(19,20)21)2(9,10)4(13,14)6(17,18)5(15,16)3(1,11)12
InchiKey:	QIROQPWSJUXOJC-UHFFFAOYSA-N
Formula:	C7F14
SMILES:	FC(F)(F)C1(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C1(F)F
Mol. weight [g/mol]:	350.05
CAS:	355-02-2

Physical Properties

Property code	Value	Unit	Source
af	0.4910		KDB
chl	-1844.90 ± 0.46	kJ/mol	NIST Webbook
ea	1.06 ± 0.13	eV	NIST Webbook
ea	1.02 ± 0.06	eV	NIST Webbook
gf	-2763.48	kJ/mol	Joback Method
hf	-2898.00	kJ/mol	KDB
hf	-2897.20 ± 3.80	kJ/mol	NIST Webbook
hfl	-2931.10 ± 3.80	kJ/mol	NIST Webbook
hfus	8.99	kJ/mol	Joback Method
hvap	34.00	kJ/mol	NIST Webbook
hvap	34.10 ± 0.30	kJ/mol	NIST Webbook
hvap	33.90 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.85		Crippen Method
logp	4.447		Crippen Method
mcvol	123.410	ml/mol	McGowan Method

pc	2018.71 ± 10.00	kPa	NIST Webbook
pc	2019.00	kPa	KDB
pc	2019.00 ± 3.00	kPa	NIST Webbook
pc	2019.00 ± 3.00	kPa	NIST Webbook
pc	2019.00 ± 3.00	kPa	NIST Webbook
pc	2019.00 ± 3.00	kPa	NIST Webbook
pc	2019.00 ± 3.00	kPa	NIST Webbook
rhoc	612.59 ± 7.00	kg/m3	NIST Webbook
rinpol	290.00		NIST Webbook
rinpol	303.00		NIST Webbook
tb	349.50	K	KDB
tb	349.20 ± 2.00	K	NIST Webbook
tb	349.55 ± 0.40	K	NIST Webbook
tb	349.53 ± 0.20	K	NIST Webbook
tb	349.56 ± 0.10	K	NIST Webbook
tb	349.30	K	NIST Webbook
tb	349.00	K	NIST Webbook
tc	485.91	K	KDB
tf	228.40	K	KDB
vc	0.570	m3/kmol	KDB
zc	0.2848520		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.00	J/mol×K	449.88	Joback Method
cpg	297.96	J/mol×K	364.98	Joback Method
cpg	312.25	J/mol×K	386.20	Joback Method
cpg	325.11	J/mol×K	407.43	Joback Method
cpg	356.24	J/mol×K	471.11	Joback Method
cpg	336.66	J/mol×K	428.66	Joback Method
cpg	282.13	J/mol×K	343.75	Joback Method
cpl	353.10	J/mol×K	298.00	NIST Webbook

dvisc	0.0009582	Pa×s	323.18	Shear Viscosities of Methycyclohexane, Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isopleth and Coexistence Curve
dvisc	0.0010114	Pa×s	320.16	Shear Viscosities of Methycyclohexane, Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isopleth and Coexistence Curve
dvisc	0.0010313	Pa×s	319.20	Shear Viscosities of Methycyclohexane, Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isopleth and Coexistence Curve
dvisc	0.0008074	Pa×s	333.11	Shear Viscosities of Methycyclohexane, Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isopleth and Coexistence Curve
dvisc	0.0008787	Pa×s	328.13	Shear Viscosities of Methycyclohexane, Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isopleth and Coexistence Curve

hsubt	51.60	kJ/mol	234.00	NIST Webbook
hvapt	33.10	kJ/mol	359.50	NIST Webbook
hvapt	30.20	kJ/mol	450.50	NIST Webbook
hvapt	33.40	kJ/mol	345.00	NIST Webbook
hvapt	33.30	kJ/mol	345.00	NIST Webbook
hvapt	33.30	kJ/mol	310.50	NIST Webbook
hvapt	33.80	kJ/mol	325.50	NIST Webbook
kvisc	0.0000009	m2/s	298.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000008	m2/s	303.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000008	m2/s	308.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000007	m2/s	313.15	Viscosities of Liquid Fluorocompounds
kvisc	0.0000007	m2/s	318.15	Viscosities of Liquid Fluorocompounds
rhol	1758.70	kg/m3	308.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1730.30	kg/m3	318.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1715.80	kg/m3	323.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K

rhol	1701.20	kg/m3	328.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1686.40	kg/m3	333.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1671.50	kg/m3	338.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1789.00	kg/m3	298.00	KDB
rhol	1841.00	kg/m3	278.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1827.60	kg/m3	283.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1814.00	kg/m3	288.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K

rhol	1800.40	kg/m3	293.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1786.60	kg/m3	298.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1772.70	kg/m3	303.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1656.30	kg/m3	343.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
rhol	1744.50	kg/m3	313.15	Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K
srf	0.02	N/m	286.75	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	308.55	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	303.35	Surface Tension of Liquid Fluorocompounds
srf	0.02	N/m	298.35	Surface Tension of Liquid Fluorocompounds

srf	0.02	N/m	293.25	Surface Tension of Liquid Fluorocompounds
srf	0.01	N/m	313.65	Surface Tension of Liquid Fluorocompounds

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.17838e+01
Coeff. B	-2.34793e+03
Coeff. C	-5.20770e+01
Temperature range (K), min.	252.15
Temperature range (K), max.	414.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.96012e+02
Coeff. B	-1.49161e+04
Coeff. C	-4.34642e+01
Coeff. D	4.72597e-05
Temperature range (K), min.	306.00
Temperature range (K), max.	483.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C355022&Units=SI
Experimental Data on Binary and Ternary Mixtures of Perfluoromethylcyclohexane with Methylcyclohexane and n-Octane at 373.15 K:	https://www.doi.org/10.1021/je049550t
Steam Viscosities of Perfluoromethylcyclohexane, and Their Mixtures in the Vicinity of the Upper Critical Mixing Temperature. 1. Critical Isochore and Coexistence Curve:	https://www.doi.org/10.1021/je0502593
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Viscosities of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je700632z
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1760
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1760.mol
Liquid Liquid Equilibria in Ternary Systems of Hexafluoroisopropanol + Perfluorocarbon + Water or Methanol at 298.15 K:	https://www.doi.org/10.1021/je500455u
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1760
Surface Tension of Liquid Fluorocompounds:	https://www.doi.org/10.1021/je060199g

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
hsubt:	Enthalpy of sublimation 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
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility

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