Methane, trifluoroiodo-

Other names:	CF3I
	CIF3
	Iodotrifluoromethane
	Perfluoromethyl iodide
	Trifluoriodomethane
	Trifluoroiodomethane
	Trifluoromethyl iodide
Inchi:	InChI=1S/CF3I/c2-1(3,4)5
InchiKey:	VPAYJEUHKVESSD-UHFFFAOYSA-N
Formula:	CF3I
SMILES:	FC(F)(F)I
Mol. weight [g/mol]:	195.91
CAS:	2314-97-8

Physical Properties

Property code	Value	Unit	Source
affp	628.00	kJ/mol	NIST Webbook
basg	598.20	kJ/mol	NIST Webbook
chg	-71.55 ± 0.71	kJ/mol	NIST Webbook
ea	2.20 ± 0.20	eV	NIST Webbook
ea	1.40 ± 0.20	eV	NIST Webbook
ea	1.57 ± 0.20	eV	NIST Webbook
gf	-565.93	kJ/mol	Joback Method
hf	-587.80 ± 3.20	kJ/mol	NIST Webbook
hfus	4.58	kJ/mol	Joback Method
hvap	23.45	kJ/mol	Joback Method
ie	10.50 ± 0.10	eV	NIST Webbook
ie	10.64 ± 0.02	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.45 ± 0.05	eV	NIST Webbook
ie	10.23	eV	NIST Webbook
ie	10.28 ± 0.07	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
ie	10.00 ± 0.30	eV	NIST Webbook
ie	10.38 ± 0.02	eV	NIST Webbook
ie	10.32 ± 0.03	eV	NIST Webbook
log10ws	-2.35		Crippen Method

logp	1.941		Crippen Method
mcvol	56.080	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
tb	250.60	K	NIST Webbook
tb	250.60	K	NIST Webbook
tc	494.44	K	Joback Method
tf	163.28	K	Joback Method
vc	0.223	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.53	J/mol×K	494.44	Joback Method
cpg	87.41	J/mol×K	463.70	Joback Method
cpg	85.00	J/mol×K	432.96	Joback Method
cpg	82.27	J/mol×K	402.22	Joback Method
cpg	79.22	J/mol×K	371.48	Joback Method
cpg	75.80	J/mol×K	340.74	Joback Method
cpg	72.01	J/mol×K	310.00	Joback Method
hvapt	22.50	kJ/mol	242.00	NIST Webbook
pvap	367.60	kPa	288.15	(Vapour + liquid) equilibrium data for the binary system of {trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))} at various temperatures from (258.150 to 298.150) K
pvap	491.70	kPa	298.15	(Vapour + liquid) equilibrium data for the binary system of {trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))} at various temperatures from (258.150 to 298.150) K

pvap	160.40	kPa	263.15	Measurements of (vapour + liquid) equilibrium data for {trifluoroiodomethane (R13I1) + isobutane (R600a)} at temperatures between (263.150 and 293.150) K
pvap	228.40	kPa	273.15	Measurements of (vapour + liquid) equilibrium data for {trifluoroiodomethane (R13I1) + isobutane (R600a)} at temperatures between (263.150 and 293.150) K
pvap	316.50	kPa	283.15	Measurements of (vapour + liquid) equilibrium data for {trifluoroiodomethane (R13I1) + isobutane (R600a)} at temperatures between (263.150 and 293.150) K
pvap	428.00	kPa	293.15	Measurements of (vapour + liquid) equilibrium data for {trifluoroiodomethane (R13I1) + isobutane (R600a)} at temperatures between (263.150 and 293.150) K
pvap	133.00	kPa	258.15	(Vapor + liquid) phase equilibrium measurements for {trifluoroiodomethane (R13I1) + propane (R290)} from T = (258.150 to 283.150) K

pvap	160.40	kPa	263.15	(Vapor + liquid) phase equilibrium measurements for {trifluoroiodomethane (R13I1) + propane (R290)} from T = (258.150 to 283.150) K
pvap	228.40	kPa	273.15	(Vapor + liquid) phase equilibrium measurements for {trifluoroiodomethane (R13I1) + propane (R290)} from T = (258.150 to 283.150) K
pvap	316.50	kPa	283.15	(Vapor + liquid) phase equilibrium measurements for {trifluoroiodomethane (R13I1) + propane (R290)} from T = (258.150 to 283.150) K
pvap	133.00	kPa	258.15	Measurements of isothermal (vapor + liquid) phase equilibrium for {trifluoroiodomethane (R13I1) + 1,1-difluoroethane (R152a)} from T = (258.150 to 283.150) K
pvap	268.40	kPa	278.15	(Vapour + liquid) equilibrium data for the binary system of {trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))} at various temperatures from (258.150 to 298.150) K
pvap	228.40	kPa	273.15	Measurements of isothermal (vapor + liquid) phase equilibrium for {trifluoroiodomethane (R13I1) + 1,1-difluoroethane (R152a)} from T = (258.150 to 283.150) K

pvap	316.50	kPa	283.15	Measurements of isothermal (vapor + liquid) phase equilibrium for {trifluoroiodomethane (R13I1) + 1,1-difluoroethane (R152a)} from T = (258.150 to 283.150) K
pvap	72.70	kPa	243.15	Experimental research on (vapor + liquid) equilibria for the {trifluoroiodomethane (CF3I) + carbon dioxide (CO2)} system from 243.150 to 273.150 K
pvap	110.10	kPa	253.15	Experimental research on (vapor + liquid) equilibria for the {trifluoroiodomethane (CF3I) + carbon dioxide (CO2)} system from 243.150 to 273.150 K
pvap	160.40	kPa	263.15	Experimental research on (vapor + liquid) equilibria for the {trifluoroiodomethane (CF3I) + carbon dioxide (CO2)} system from 243.150 to 273.150 K
pvap	228.40	kPa	273.15	Experimental research on (vapor + liquid) equilibria for the {trifluoroiodomethane (CF3I) + carbon dioxide (CO2)} system from 243.150 to 273.150 K
pvap	71.70	kPa	243.15	Vapor Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K

pvap	109.00	kPa	253.15	Vapor Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K
pvap	160.40	kPa	263.15	Vapor Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K
pvap	228.20	kPa	273.15	Vapor Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K
pvap	316.30	kPa	283.15	Vapor Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K
pvap	191.10	kPa	268.15	(Vapour + liquid) equilibrium data for the binary system of {trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))} at various temperatures from (258.150 to 298.150) K

pvap	132.00	kPa	258.15	(Vapour + liquid) equilibrium data for the binary system of {trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))} at various temperatures from (258.150 to 298.150) K
pvap	316.40	kPa	283.15	Phase equilibrium for the binary azeotropic mixture of trifluoroiodomethane (R13I1) + 1,1,2,2-tetrafluoroethane (R134) at temperatures from 258.150 to 283.150 K
pvap	228.40	kPa	273.15	Phase equilibrium for the binary azeotropic mixture of trifluoroiodomethane (R13I1) + 1,1,2,2-tetrafluoroethane (R134) at temperatures from 258.150 to 283.150 K
pvap	160.40	kPa	263.15	Phase equilibrium for the binary azeotropic mixture of trifluoroiodomethane (R13I1) + 1,1,2,2-tetrafluoroethane (R134) at temperatures from 258.150 to 283.150 K
pvap	133.00	kPa	258.15	Phase equilibrium for the binary azeotropic mixture of trifluoroiodomethane (R13I1) + 1,1,2,2-tetrafluoroethane (R134) at temperatures from 258.150 to 283.150 K

pvap	160.40	kPa	263.15	Measurements of isothermal (vapor + liquid) phase equilibrium for {trifluoroiodomethane (R13I1) + 1,1-difluoroethane (R152a)} from T = (258.150 to 283.150) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53780e+01
Coeff. B	-2.70390e+03
Temperature range (K), min.	179.18
Temperature range (K), max.	396.44

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
298.15	2000.00	2046.84

Reference *https://www.doi.org/10.1021/je3008974*

Sources

(Vapor + liquid) phase equilibrium measurements for {trifluoroiodomethane (R13I1) + propane (R290)} from T = (258.150 to 283.150) K:	https://www.doi.org/10.1016/j.jct.2014.07.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor-Liquid Phase Equilibrium for Azeotropic Isobutane + trans-1,3,3,3-Tetrafluoropropene + Trifluoroiodomethane System at Temperatures from 243.150 to 283.150 K:	https://www.doi.org/10.1021/acs.jced.7b00964
Gaseous PVT measurements for propane (R290) + trifluoroiodomethane (R13I1) system:	https://www.doi.org/10.1016/j.fluid.2019.04.033

(Vapour + liquid) equilibrium data for the binary system of (trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))) at various temperatures from 258.150 to 308.150 K:	https://www.doi.org/10.1016/j.jct.2011.11.024
Experimental research on (vapor + liquid) equilibria for the (trifluoroiodomethane (R13I1) + trans-1, 3, 3, 3-tetrafluoropropene (R1234ze (E))) at various temperatures from 258.150 to 308.150 K:	https://www.doi.org/10.1016/j.jct.2016.05.012
Phase equilibrium for the binary azeotropic mixtures of (trifluoroiodomethane (R13I1) + trans-1,3,3,3-Tetrafluoropropene (R1234ze(E))):	https://www.doi.org/10.1016/j.fluid.2011.11.013
Isothermal Vapor-Liquid Measurements for (trifluoroiodomethane (R13I1) + 1,1,2,2-tetrafluoroethane (R134)) at temperatures from 258.150 to 283.150 K:	https://www.doi.org/10.1021/je3008974
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Trifluorojodomethane (R13I1) at Temperatures from (205 to 353) K under Pressures up to 40 MPa:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurements of Isothermal (Vapor + liquid) phase equilibrium for (trifluoroiodomethane (R13I1) + 1,1-difluoroethane (R152a)} from T = (258.150 to 283.150) K:	https://www.doi.org/10.1016/j.jct.2015.04.011
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2314978&Units=SI
Measurements of (vapour + liquid) equilibrium data for (trifluoroiodomethane (R13I1) + isobutane (R600a)} at temperatures between (263.150 and 293.150) K:	https://www.doi.org/10.1016/j.jct.2012.10.003
McGowan 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

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume