Methane, iodo-

Other names:	CH3I
	HALON 10001
	IODOMETHANE
	Iodometano
	Iodure de methyle
	Jod-methan
	Joodmethaan
	METHYL IODIDE
	Methyl iodine
	Methyljodid
	Methyljodide
	Metylu jodek
	Monoiodomethane
	Monoioduro di metile
	NSC 9366
	Rcra waste number U138
	UN 2644
Inchi:	InChI=1S/CH3I/c1-2/h1H3
InchiKey:	INQOMBQAUSQDDS-UHFFFAOYSA-N
Formula:	CH3I
SMILES:	CI
Mol. weight [g/mol]:	141.94
CAS:	74-88-4

Physical Properties

Property code	Value	Unit	Source
af	0.1380		KDB
affp	691.70	kJ/mol	NIST Webbook
basg	665.50	kJ/mol	NIST Webbook
chl	-808.60 ± 0.30	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
ea	0.30 ± 0.20	eV	NIST Webbook
ea	0.11 ± 0.02	eV	NIST Webbook
gf	15.66	kJ/mol	KDB
hf	16.00 ± 1.00	kJ/mol	NIST Webbook
hf	14.60 ± 1.00	kJ/mol	NIST Webbook
hf	14.30 ± 1.40	kJ/mol	NIST Webbook

hf	13.98	kJ/mol	KDB
hfl	-13.60 ± 0.50	kJ/mol	NIST Webbook
hfl	-12.00 ± 1.00	kJ/mol	NIST Webbook
hfus	2.75	kJ/mol	Joback Method
hvap	27.19	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	10.14	eV	NIST Webbook
ie	9.51	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
ie	9.54 ± 0.00	eV	NIST Webbook
ie	9.53 ± 0.01	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.54 ± 0.02	eV	NIST Webbook
ie	9.54 ± 0.05	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	10.86	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.53 ± 0.01	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.48 ± 0.03	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
log10ws	-1.00		Estimated Solubility Method
log10ws	-1.00		Aqueous Solubility Prediction Method
logp	1.051		Crippen Method
mcvol	50.770	ml/mol	McGowan Method
pc	6590.00	kPa	KDB
rinpol	513.00		NIST Webbook
rinpol	528.60		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	509.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	523.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	506.00		NIST Webbook
rinpol	554.00		NIST Webbook

rinpol	516.00		NIST Webbook
rinpol	502.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	528.00		NIST Webbook
rinpol	508.00		NIST Webbook
rinpol	523.00		NIST Webbook
ripol	802.99		NIST Webbook
ripol	806.00		NIST Webbook
ripol	806.00		NIST Webbook
ripol	818.02		NIST Webbook
ripol	804.33		NIST Webbook
ripol	833.00		NIST Webbook
tb	315.70	K	KDB
tc	528.00	K	KDB
tf	206.70	K	KDB
tf	207.30	K	Aqueous Solubility Prediction Method
tf	206.70 ± 0.50	K	NIST Webbook
tf	208.10 ± 0.40	K	NIST Webbook
vc	0.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	47.27	J/mol×K	315.42	Joback Method
cpg	56.92	J/mol×K	453.44	Joback Method
cpg	54.74	J/mol×K	418.94	Joback Method
cpg	52.41	J/mol×K	384.43	Joback Method
cpg	60.89	J/mol×K	522.45	Joback Method
cpg	49.92	J/mol×K	349.93	Joback Method
cpg	58.97	J/mol×K	487.95	Joback Method
cpl	82.75	J/mol×K	298.15	NIST Webbook
cpl	82.00	J/mol×K	298.15	NIST Webbook
cpl	82.76	J/mol×K	298.20	NIST Webbook
cpl	82.68	J/mol×K	300.00	NIST Webbook
cpl	148.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0006734	Pa×s	263.31	Joback Method
dvisc	0.0004180	Pa×s	315.42	Joback Method
dvisc	0.0005193	Pa×s	289.37	Joback Method
dvisc	0.0009245	Pa×s	237.25	Joback Method

dvisc	0.0013726	Pa×s	211.20	Joback Method
dvisc	0.0022777	Pa×s	185.15	Joback Method
dvisc	0.0044613	Pa×s	159.09	Joback Method
hfust	9.12	kJ/mol	206.80	NIST Webbook
hfust	9.10	kJ/mol	206.80	NIST Webbook
hsubt	40.20 ± 0.40	kJ/mol	201.50	NIST Webbook
hvapt	26.50	kJ/mol	408.50	NIST Webbook
hvapt	31.10	kJ/mol	217.50	NIST Webbook
hvapt	29.20	kJ/mol	286.50	NIST Webbook
hvapt	30.40	kJ/mol	266.50	NIST Webbook
hvapt	28.20	kJ/mol	290.00	NIST Webbook
hvapt	28.41	kJ/mol	315.80	NIST Webbook
hvapt	27.20	kJ/mol	315.60	KDB
hvapt	30.40	kJ/mol	282.50	NIST Webbook
pvap	69.90	kPa	303.15	Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I)
pvap	95.00	kPa	313.15	Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I)
pvap	129.00	kPa	323.15	Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I)
pvap	30.00	kPa	283.15	Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I)
pvap	47.50	kPa	293.15	Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I)
rhol	2279.00	kg/m3	293.00	KDB
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48574e+01
Coeff. B	-3.02828e+03
Coeff. C	-1.99430e+01
Temperature range (K), min.	206.70
Temperature range (K), max.	337.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.75767e+01
Coeff. B	-5.02586e+03
Coeff. C	-6.54993e+00
Coeff. D	6.60013e-06
Temperature range (K), min.	206.70
Temperature range (K), max.	528.00

Sources

KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1532
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isothermal vapor-liquid equilibria for the binary system of dimethylether (DME) + methyl iodide (CH3I):	https://www.doi.org/10.1016/j.fluid.2014.06.029
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74884&Units=SI
Determination of Henry's Law Constants Using Internal Standards With Benchmark Values:	https://www.doi.org/10.1021/je3010535
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1532
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1532
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume