Ethane, iodo-

Other names:	1-Iodoethane
	C2H5I
	ETHYL IODIDE
	Ethyljodid
	HYDRIODIC ETHER
	Iodoethane
	Jodethan
	Monoiodoethane
	NSC 8825
Inchi:	InChI=1S/C2H5I/c1-2-3/h2H2,1H3
InchiKey:	HVTICUPFWKNHNG-UHFFFAOYSA-N
Formula:	C2H5I
SMILES:	CCI
Mol. weight [g/mol]:	155.97
CAS:	75-03-6

Physical Properties

Property code	Value	Unit	Source
af	0.1840		KDB
affp	724.80	kJ/mol	NIST Webbook
basg	698.30	kJ/mol	NIST Webbook
chl	-1466.00 ± 2.00	kJ/mol	NIST Webbook
chl	-1462.50 ± 0.40	kJ/mol	NIST Webbook
dm	1.70	debye	KDB
gf	21.35	kJ/mol	KDB
gyrad	0.2775		KDB
hf	-8.40	kJ/mol	NIST Webbook
hf	-7.20 ± 0.80	kJ/mol	NIST Webbook
hf	-8.37	kJ/mol	KDB
hf	-5.40	kJ/mol	NIST Webbook
hf	-8.80 ± 0.80	kJ/mol	NIST Webbook
hfl	-39.10 ± 0.80	kJ/mol	NIST Webbook
hfl	-35.00	kJ/mol	NIST Webbook
hfl	-39.50 ± 1.70	kJ/mol	NIST Webbook
hfus	5.34	kJ/mol	Joback Method
hvap	31.70	kJ/mol	NIST Webbook
hvap	31.90 ± 0.10	kJ/mol	NIST Webbook

hvap	31.93 ± 0.02	kJ/mol	NIST Webbook
hvap	29.80 ± 0.30	kJ/mol	NIST Webbook
hvap	32.05	kJ/mol	NIST Webbook
ie	9.35 ± 0.01	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.45 ± 0.02	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.35 ± 0.00	eV	NIST Webbook
ie	9.35 ± 0.00	eV	NIST Webbook
ie	9.33 ± 0.01	eV	NIST Webbook
ie	9.35 ± 0.02	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
ie	9.35 ± 0.02	eV	NIST Webbook
ie	9.35 ± 0.01	eV	NIST Webbook
ie	9.35	eV	NIST Webbook
log10ws	-1.60		Estimated Solubility Method
log10ws	-1.60		Aqueous Solubility Prediction Method
logp	1.441		Crippen Method
mcvol	64.860	ml/mol	McGowan Method
pc	4700.00	kPa	KDB
rinpol	600.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	621.00		NIST Webbook
rinpol	607.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	617.60		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	598.00		NIST Webbook
rinpol	609.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	616.00		NIST Webbook

rinpol	602.00		NIST Webbook
rinpol	601.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	586.00		NIST Webbook
ripol	881.00		NIST Webbook
ripol	899.84		NIST Webbook
ripol	896.49		NIST Webbook
ripol	892.00		NIST Webbook
ripol	901.65		NIST Webbook
ripol	876.00		NIST Webbook
ripol	881.00		NIST Webbook
ripol	892.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	901.65		NIST Webbook
tb	345.40 ± 1.00	K	NIST Webbook
tb	344.20	K	NIST Webbook
tb	345.50	K	NIST Webbook
tb	345.60	K	NIST Webbook
tb	345.60	K	KDB
tb	345.45 ± 0.40	K	NIST Webbook
tb	346.35 ± 0.30	K	NIST Webbook
tb	345.45 ± 0.25	K	NIST Webbook
tb	345.50 ± 0.50	K	NIST Webbook
tb	345.52 ± 0.25	K	NIST Webbook
tb	345.85 ± 0.30	K	NIST Webbook
tb	345.50 ± 0.40	K	NIST Webbook
tb	345.50	K	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa
tb	345.57 ± 0.10	K	NIST Webbook
tc	554.00	K	KDB
tf	165.00	K	KDB
tf	163.62	K	Aqueous Solubility Prediction Method
tf	162.05 ± 0.40	K	NIST Webbook
tf	162.30 ± 0.40	K	NIST Webbook
vc	0.235	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	98.71	J/mol×K	544.92	Joback Method
cpg	74.51	J/mol×K	338.30	Joback Method
cpg	95.23	J/mol×K	510.48	Joback Method
cpg	91.55	J/mol×K	476.05	Joback Method
cpg	87.65	J/mol×K	441.61	Joback Method
cpg	83.52	J/mol×K	407.17	Joback Method
cpg	79.14	J/mol×K	372.74	Joback Method
cpl	115.10	J/mol×K	298.00	NIST Webbook
cpl	109.70	J/mol×K	298.15	NIST Webbook
dvisc	0.0006970	Pa×s	282.32	Joback Method
dvisc	0.0025088	Pa×s	198.35	Joback Method
dvisc	0.0014730	Pa×s	226.34	Joback Method
dvisc	0.0004224	Pa×s	338.30	Joback Method
dvisc	0.0005305	Pa×s	310.31	Joback Method
dvisc	0.0050904	Pa×s	170.36	Joback Method
dvisc	0.0009723	Pa×s	254.33	Joback Method
hvapt	34.70	kJ/mol	282.00	NIST Webbook
hvapt	29.44	kJ/mol	345.60	NIST Webbook
hvapt	33.60	kJ/mol	309.00	NIST Webbook
hvapt	29.77	kJ/mol	345.60	KDB
hvapt	31.70	kJ/mol	318.00	NIST Webbook
hvapt	32.00	kJ/mol	273.50	NIST Webbook
pvap	101.30	kPa	345.50	Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa
rfi	1.50950		298.15	Experimental and predicted volumetric and refractive index properties of ternary mixtures of iodoethane with toluene and alcohols at temperature 298.15 K and pressure 101 kPa
rhol	1950.00	kg/m3	293.00	KDB

rhol	1923.80	kg/m3	298.15	Solubility and Liquid-Liquid Equilibrium of Aqueous Systems of Iodoethane with Methanol, Ethanol, or 1-Propanol at Temperature 298.15 K and Pressure 101.2 kPa
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45544e+01
Coeff. B	-3.07804e+03
Coeff. C	-3.57160e+01
Temperature range (K), min.	251.46
Temperature range (K), max.	368.73

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.81996e+01
Coeff. B	-5.85116e+03
Coeff. C	-8.13893e+00
Coeff. D	7.75920e-06
Temperature range (K), min.	162.05
Temperature range (K), max.	561.00

Sources

Solubility and Liquid-Liquid Equilibrium of Aqueous Systems of Iodoethane with Methanol, Ethanol, or 1-Propanol at Temperature 298.15 K and Pressure 101.2 kPa:	https://www.doi.org/10.1021/je900059e
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Isobaric vapour-liquid equilibrium for binary systems of ethyl iodide with ethanol, propionic acid and ethyl propionate at 101.3 kPa:	https://www.doi.org/10.1016/j.jct.2018.12.023

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75036&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental and predicted volumetric and refractive index properties of ternary mixtures of iodoethane with toluene and alcohols at temperature 298.15 K and pressure 101 kPa:	https://www.doi.org/10.1016/j.jct.2005.05.004
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1580
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1580.mol
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rfi:	Refractive Index
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