Propane, 1-iodo-

Other names:	1-Iodopropane
	1-Jodpropan
	N-PROPYL IODIDE
	Propyl iodide
	n-C3H7I
Inchi:	InChI=1S/C3H7I/c1-2-3-4/h2-3H2,1H3
InchiKey:	PVWOIHVRPOBWPI-UHFFFAOYSA-N
Formula:	C3H7I
SMILES:	CCCI
Mol. weight [g/mol]:	169.99
CAS:	107-08-4

Physical Properties

Property code	Value	Unit	Source
af	0.2240		KDB
gf	32.50	kJ/mol	Joback Method
hf	-31.00	kJ/mol	NIST Webbook
hfl	-65.70 ± 3.00	kJ/mol	NIST Webbook
hfus	7.93	kJ/mol	Joback Method
hvap	36.25 ± 0.04	kJ/mol	NIST Webbook
hvap	36.32	kJ/mol	NIST Webbook
hvap	36.30 ± 0.10	kJ/mol	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
ie	9.27	eV	NIST Webbook
ie	9.27	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.25 ± 0.01	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
ie	9.27	eV	NIST Webbook
ie	9.27	eV	NIST Webbook
ie	9.26 ± 0.01	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.26	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	9.25	eV	NIST Webbook

log10ws	-2.29		Aqueous Solubility Prediction Method
log10ws	-2.29		Estimated Solubility Method
logp	1.831		Crippen Method
mcvol	78.950	ml/mol	McGowan Method
pc	4280.00	kPa	KDB
rinpol	715.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	719.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	720.30		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	702.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	719.00		NIST Webbook
ripol	971.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	975.00		NIST Webbook
tb	375.60	K	KDB
tc	589.40	K	KDB
tf	171.75 ± 0.30	K	NIST Webbook
tf	172.00	K	KDB
tf	172.07	K	Aqueous Solubility Prediction Method
vc	0.291	m3/kmol	KDB
zc	0.2545870		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.46	J/mol×K	566.82	Joback Method
cpg	110.94	J/mol×K	395.45	Joback Method
cpg	117.06	J/mol×K	429.73	Joback Method
cpg	122.86	J/mol×K	464.00	Joback Method
cpg	128.34	J/mol×K	498.28	Joback Method
cpg	133.54	J/mol×K	532.55	Joback Method

cpg	104.48	J/mol×K	361.18	Joback Method
cpl	126.80	J/mol×K	298.00	NIST Webbook
cpl	136.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0055945	Pa×s	181.63	Joback Method
dvisc	0.0026731	Pa×s	211.56	Joback Method
dvisc	0.0015337	Pa×s	241.48	Joback Method
dvisc	0.0009947	Pa×s	271.40	Joback Method
dvisc	0.0007031	Pa×s	301.33	Joback Method
dvisc	0.0004174	Pa×s	361.18	Joback Method
dvisc	0.0005291	Pa×s	331.25	Joback Method
hvapt	35.43	kJ/mol	375.60	KDB
hvapt	32.08	kJ/mol	375.70	NIST Webbook
hvapt	37.80	kJ/mol	221.00	NIST Webbook
hvapt	36.80	kJ/mol	336.50	NIST Webbook
hvapt	37.00	kJ/mol	306.00	NIST Webbook
rhol	1802.50	kg/m3	263.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1820.90	kg/m3	253.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1784.50	kg/m3	273.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1765.90	kg/m3	283.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1747.80	kg/m3	293.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K

rhol	1688.30	kg/m3	324.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1652.20	kg/m3	343.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K
rhol	1622.30	kg/m3	358.15	Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48622e+01
Coeff. B	-3.60870e+03
Coeff. C	-2.32210e+01
Temperature range (K), min.	270.82
Temperature range (K), max.	401.20

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.29299e+01
Coeff. B	-7.25894e+03
Coeff. C	-1.18977e+01
Coeff. D	1.09325e-05
Temperature range (K), min.	171.15
Temperature range (K), max.	593.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1598
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C107084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Density of 1-Iodopropane and 1-Iodobutane within the Temperature Range from (253.15 to 383.15) K:	https://www.doi.org/10.1021/je700020t
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1598.mol

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility