Propane, 2-iodo-

Other names:	2-Iodopropane
	2-Jodpropan
	ISOPROPYL IODIDE
	Isopropyl iodine
	Propane, iodo-
	SEC-PROPYL IODIDE
	i-Propyl iodide
	iso-C3H7I
Inchi:	InChI=1S/C3H7I/c1-3(2)4/h3H,1-2H3
InchiKey:	FMKOJHQHASLBPH-UHFFFAOYSA-N
Formula:	C3H7I
SMILES:	CC(C)I
Mol. weight [g/mol]:	169.99
CAS:	75-30-9

Physical Properties

Property code	Value	Unit	Source
af	0.1950		KDB
gf	30.06	kJ/mol	Joback Method
hf	-33.66	kJ/mol	Joback Method
hfl	-74.90 ± 2.30	kJ/mol	NIST Webbook
hfus	4.41	kJ/mol	Joback Method
hvap	34.06 ± 0.06	kJ/mol	NIST Webbook
hvap	34.14	kJ/mol	NIST Webbook
hvap	34.00	kJ/mol	NIST Webbook
hvap	34.10 ± 0.10	kJ/mol	NIST Webbook
ie	9.20 ± 0.10	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.18 ± 0.01	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.19	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.40	eV	NIST Webbook

ie	9.19 ± 0.02	eV	NIST Webbook
ie	9.15	eV	NIST Webbook
ie	9.17 ± 0.02	eV	NIST Webbook
ie	9.19 ± 0.02	eV	NIST Webbook
log10ws	-2.09		Aqueous Solubility Prediction Method
log10ws	-2.09		Estimated Solubility Method
logp	1.830		Crippen Method
mcvol	78.950	ml/mol	McGowan Method
pc	4330.00	kPa	KDB
rinpol	670.00		NIST Webbook
rinpol	654.00		NIST Webbook
rinpol	661.00		NIST Webbook
tb	362.00 ± 1.00	K	NIST Webbook
tb	362.10 ± 2.00	K	NIST Webbook
tb	362.20 ± 1.50	K	NIST Webbook
tb	362.65 ± 0.10	K	NIST Webbook
tb	362.60	K	NIST Webbook
tb	362.60	K	NIST Webbook
tb	362.60	K	KDB
tb	362.50 ± 0.50	K	NIST Webbook
tc	574.60	K	KDB
tf	182.40 ± 0.30	K	NIST Webbook
tf	183.15 ± 0.40	K	NIST Webbook
tf	183.00	K	KDB
tf	180.10 ± 2.00	K	NIST Webbook
vc	0.285	m3/kmol	KDB
zc	0.2587570		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.25	J/mol×K	501.40	Joback Method
cpg	123.56	J/mol×K	466.24	Joback Method
cpg	139.70	J/mol×K	571.73	Joback Method
cpg	134.62	J/mol×K	536.57	Joback Method
cpg	104.41	J/mol×K	360.74	Joback Method
cpg	111.15	J/mol×K	395.91	Joback Method
cpg	117.53	J/mol×K	431.07	Joback Method
cpl	137.30	J/mol×K	298.15	NIST Webbook
dvisc	0.0004067	Pa×s	360.74	Joback Method

dvisc	0.0011123	Pa×s	263.69	Joback Method
dvisc	0.0007391	Pa×s	296.04	Joback Method
dvisc	0.0005323	Pa×s	328.39	Joback Method
dvisc	0.0098235	Pa×s	166.63	Joback Method
dvisc	0.0037530	Pa×s	198.98	Joback Method
dvisc	0.0018766	Pa×s	231.33	Joback Method
hvapt	36.30	kJ/mol	296.50	NIST Webbook
hvapt	36.70	kJ/mol	217.50	NIST Webbook
hvapt	30.68	kJ/mol	362.60	NIST Webbook
hvapt	34.49	kJ/mol	362.60	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46020e+01
Coeff. B	-3.30599e+03
Coeff. C	-3.12600e+01
Temperature range (K), min.	262.22
Temperature range (K), max.	387.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.20861e+02
Coeff. B	-8.05092e+03
Coeff. C	-1.63330e+01
Coeff. D	1.66867e-05
Temperature range (K), min.	173.15
Temperature range (K), max.	578.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=1599

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1599.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75309&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility