Propane, 1-iodo-2-methyl-

Other names:	1-Iodo-2-methylpropane
	1-Jod-2-methylpropan
	Isobutyl iodide
	Isobutyljodid
	Primary isobutyl iodide
	iso-C4H9I
Inchi:	InChI=1S/C4H9I/c1-4(2)3-5/h4H,3H2,1-2H3
InchiKey:	BTUGGGLMQBJCBN-UHFFFAOYSA-N
Formula:	C4H9I
SMILES:	CC(C)CI
Mol. weight [g/mol]:	184.02
CAS:	513-38-2

Physical Properties

Property code	Value	Unit	Source
gf	38.48	kJ/mol	Joback Method
hf	-54.30	kJ/mol	Joback Method
hfus	7.00	kJ/mol	Joback Method
hvap	38.83 ± 0.02	kJ/mol	NIST Webbook
hvap	38.80 ± 0.10	kJ/mol	NIST Webbook
hvap	38.86	kJ/mol	NIST Webbook
ie	9.08	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.18 ± 0.01	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.04	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.18 ± 0.01	eV	NIST Webbook
ie	9.18 ± 0.02	eV	NIST Webbook
log10ws	-2.20		Crippen Method
logp	2.077		Crippen Method
mcvol	93.040	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	759.00		NIST Webbook

rinpol	767.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	779.00		NIST Webbook
tb	393.60 ± 0.50	K	NIST Webbook
tb	393.20	K	NIST Webbook
tb	394.20	K	NIST Webbook
tb	393.00 ± 2.00	K	NIST Webbook
tb	393.60 ± 0.50	K	NIST Webbook
tc	593.02	K	Joback Method
tf	169.00 ± 0.40	K	NIST Webbook
tf	169.15 ± 0.40	K	NIST Webbook
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.04	J/mol×K	383.62	Joback Method
cpg	145.49	J/mol×K	418.52	Joback Method
cpg	153.49	J/mol×K	453.42	Joback Method
cpg	161.06	J/mol×K	488.32	Joback Method
cpg	168.23	J/mol×K	523.22	Joback Method
cpg	175.01	J/mol×K	558.12	Joback Method
cpg	181.41	J/mol×K	593.02	Joback Method
cpl	165.50	J/mol×K	298.15	NIST Webbook
cpl	162.30	J/mol×K	298.00	NIST Webbook
dvisc	0.0005165	Pa×s	349.33	Joback Method
dvisc	0.0007232	Pa×s	315.05	Joback Method
dvisc	0.0010993	Pa×s	280.76	Joback Method
dvisc	0.0018774	Pa×s	246.47	Joback Method
dvisc	0.0038120	Pa×s	212.19	Joback Method
dvisc	0.0003918	Pa×s	383.62	Joback Method
dvisc	0.0101698	Pa×s	177.90	Joback Method
hvapt	41.10	kJ/mol	324.50	NIST Webbook
hvapt	33.54	kJ/mol	394.20	NIST Webbook
pvap	0.65	kPa	273.31	Vapor Pressure of Selected Organic Iodides
pvap	0.88	kPa	278.35	Vapor Pressure of Selected Organic Iodides
pvap	0.88	kPa	278.35	Vapor Pressure of Selected Organic Iodides

pvap	0.47	kPa	268.37	Vapor Pressure of Selected Organic Iodides
pvap	1.20	kPa	283.39	Vapor Pressure of Selected Organic Iodides
pvap	1.20	kPa	283.39	Vapor Pressure of Selected Organic Iodides
pvap	1.60	kPa	288.35	Vapor Pressure of Selected Organic Iodides
pvap	1.59	kPa	288.35	Vapor Pressure of Selected Organic Iodides
pvap	2.09	kPa	293.27	Vapor Pressure of Selected Organic Iodides
pvap	2.09	kPa	293.27	Vapor Pressure of Selected Organic Iodides
pvap	2.73	kPa	298.25	Vapor Pressure of Selected Organic Iodides
pvap	2.73	kPa	298.25	Vapor Pressure of Selected Organic Iodides
pvap	2.73	kPa	298.25	Vapor Pressure of Selected Organic Iodides
pvap	3.53	kPa	303.23	Vapor Pressure of Selected Organic Iodides
pvap	3.52	kPa	303.23	Vapor Pressure of Selected Organic Iodides
pvap	0.47	kPa	268.37	Vapor Pressure of Selected Organic Iodides
pvap	0.34	kPa	263.70	Vapor Pressure of Selected Organic Iodides
pvap	0.34	kPa	263.70	Vapor Pressure of Selected Organic Iodides
pvap	0.23	kPa	258.35	Vapor Pressure of Selected Organic Iodides
pvap	0.23	kPa	258.35	Vapor Pressure of Selected Organic Iodides
pvap	0.23	kPa	258.35	Vapor Pressure of Selected Organic Iodides
pvap	0.88	kPa	278.35	Vapor Pressure of Selected Organic Iodides

pvap	0.64	kPa	273.31	Vapor Pressure of Selected Organic Iodides
pvap	1.20	kPa	283.39	Vapor Pressure of Selected Organic Iodides

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.75134e+01
Coeff. B	-5.16156e+03
Coeff. C	7.07300e+00
Temperature range (K), min.	292.57
Temperature range (K), max.	415.94

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513382&Units=SI
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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Pressure of Selected Organic Iodides:	https://www.doi.org/10.1021/je100398m
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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