Iodine

Other names:	Diatomic iodine
	Diiodine
	ERANOL
	I2
	IODE
	Iodine crystals
	Iodine sublimed
	Iodine-127
	Iodio
	Iosan Superdip
	Jod
	Jood
	Molecular iodine
	Tincture iodine
	Vistarin
Inchi:	InChI=1S/I2/c1-2
InchiKey:	PNDPGZBMCMUPRI-UHFFFAOYSA-N
Formula:	I2
SMILES:	II
Mol. weight [g/mol]:	253.81
CAS:	7553-56-2

Physical Properties

Property code	Value	Unit	Source
dm	1.30	debye	KDB
ea	2.52 ± 0.01	eV	NIST Webbook
ea	2.52 ± 0.10	eV	NIST Webbook
ea	2.42 ± 0.20	eV	NIST Webbook
ea	1.72 ± 0.05	eV	NIST Webbook
ea	2.33	eV	NIST Webbook
ea	2.60 ± 0.10	eV	NIST Webbook
ea	2.40 ± 0.10	eV	NIST Webbook
ea	2.58 ± 0.10	eV	NIST Webbook
gf	19.38	kJ/mol	KDB
hf	62.42 ± 0.08	kJ/mol	NIST Webbook
hf	62.47	kJ/mol	KDB
hfus	4.57	kJ/mol	Joback Method

hvap	34.34	kJ/mol	Joback Method
ie	9.40 ± 0.00	eV	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.34	eV	NIST Webbook
ie	9.22 ± 0.01	eV	NIST Webbook
ie	9.31 ± 0.00	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.30 ± 0.05	eV	NIST Webbook
ie	9.30 ± 0.20	eV	NIST Webbook
ie	9.30 ± 0.20	eV	NIST Webbook
ie	9.30 ± 0.20	eV	NIST Webbook
ie	9.29 ± 0.05	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.31 ± 0.00	eV	NIST Webbook
ie	9.31 ± 0.00	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.36	eV	NIST Webbook
ie	9.31 ± 0.00	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	1.771		Crippen Method
mcvol	62.500	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
sgb	260.69 ± 0.01	J/mol×K	NIST Webbook
ss	116.14 ± 0.30	J/mol×K	NIST Webbook
tb	457.50	K	KDB
tc	819.00	K	KDB
tf	386.80	K	KDB
vc	0.155	m3/kmol	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	41.08	J/mol×K	385.68	Joback Method
cpg	41.20	J/mol×K	429.08	Joback Method
cpg	41.12	J/mol×K	472.49	Joback Method
cpg	40.89	J/mol×K	515.89	Joback Method
cpg	40.54	J/mol×K	559.29	Joback Method
cpg	40.10	J/mol×K	602.69	Joback Method
cpg	39.60	J/mol×K	646.10	Joback Method
dvisc	0.0057828	Pa×s	205.88	Joback Method
dvisc	0.0030790	Pa×s	235.85	Joback Method

dvisc	0.0018897	Pa×s	265.81	Joback Method
dvisc	0.0012804	Pa×s	295.78	Joback Method
dvisc	0.0009320	Pa×s	325.75	Joback Method
dvisc	0.0007156	Pa×s	355.71	Joback Method
dvisc	0.0005725	Pa×s	385.68	Joback Method
rhol	3740.00	kg/m3	453.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43503e+01
Coeff. B	-3.58505e+03
Coeff. C	-8.91800e+01
Temperature range (K), min.	242.00
Temperature range (K), max.	819.15

Sources

Experimental and computational study of the thermochemistry of the three iodonitrobenzene isomers:	https://www.doi.org/10.1016/j.jct.2012.09.031
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
Thermodynamic and aromaticity studies for the assessment of the halogen...cyano interactions on iodobenzonitrile:	https://www.doi.org/10.1016/j.jct.2013.06.003
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1955
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
A calorimetric and computational study of the thermochemistry of halogenated 1-phenylpyrrole derivatives :	https://www.doi.org/10.1016/j.jct.2010.06.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7553562&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational study of the molecular energetics of the iodomethoxybenzoate isomers:	https://www.doi.org/10.1016/j.jct.2011.12.001
Vapor-Liquid Equilibria for the HI + H2O System and the HI + H2O + I2 System:	https://www.doi.org/10.1021/je700544w

Legend

cpg:	Ideal gas 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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
sgb:	Molar entropy at standard conditions (1 bar)
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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