IODOBENZENE

Other names: Benzene iodide
benzene, iodo-
phenyl iodide
Inchi: InChI=1S/C6H5I/c7-6-4-2-1-3-5-6/h1-5H
InchiKey: SNHMUERNLJLMHN-UHFFFAOYSA-N
Formula: C6H5I
SMILES: Ic1ccccc1
Mol. weight [g/mol]: 204.01
CAS: 591-50-4

Physical Properties

Property code	Value	Unit	Source
af	0.2490		KDB
chl	-3192.80 ± 4.20	kJ/mol	NIST Webbook
chl	-3192.80 ± 4.20	kJ/mol	NIST Webbook
dm	1.40	debye	KDB
gf	187.90	kJ/mol	KDB
hf	165.00 ± 5.90	kJ/mol	NIST Webbook
hf	162.70	kJ/mol	KDB
hfl	117.00 ± 4.20	kJ/mol	NIST Webbook
hfus	9.74	kJ/mol	Joback Method
hvap	47.40	kJ/mol	NIST Webbook
hvap	48.90	kJ/mol	NIST Webbook
hvap	47.70 ± 4.20	kJ/mol	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.77 ± 0.02	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.73 ± 0.01	eV	NIST Webbook
ie	8.72 ± 0.04	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	8.79	eV	NIST Webbook
ie	8.73 ± 0.03	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
ie	9.05	eV	NIST Webbook
ie	8.70	eV	NIST Webbook

ie	8.79	eV	NIST Webbook
log10ws	-3.01		Estimated Solubility Method
log10ws	-2.89		Aqueous Solubility Prediction Method
logp	2.291		Crippen Method
mcvol	97.460	ml/mol	McGowan Method
pc	4520.00	kPa	KDB
rinpol	1088.00		NIST Webbook
rinpol	1079.60		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1079.60		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1088.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1569.00		NIST Webbook
sl	205.40	J/mol×K	NIST Webbook
tb	461.50	K	NIST Webbook
tb	461.60	K	KDB
tb	461.60 ± 0.30	K	NIST Webbook
tb	460.85 ± 0.50	K	NIST Webbook
tb	461.15 ± 0.30	K	NIST Webbook
tb	461.70 ± 0.50	K	NIST Webbook
tb	461.70 ± 0.50	K	NIST Webbook
tc	721.00	K	KDB
tf	241.80 ± 0.30	K	NIST Webbook
tf	241.90 ± 0.02	K	NIST Webbook
tf	242.15 ± 1.00	K	NIST Webbook
tf	242.05	K	Aqueous Solubility Prediction Method
tf	241.80	K	KDB
tt	241.80 ± 0.25	K	NIST Webbook
tt	241.80 ± 0.25	K	NIST Webbook
vc	0.351	m3/kmol	KDB
zc	0.2646510		KDB
zra	0.26		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.37	J/mol×K	456.50	Joback Method
cpg	190.37	J/mol×K	713.20	Joback Method
cpg	184.39	J/mol×K	670.42	Joback Method
cpg	177.81	J/mol×K	627.64	Joback Method
cpg	170.58	J/mol×K	584.85	Joback Method
cpg	162.63	J/mol×K	542.07	Joback Method
cpg	153.92	J/mol×K	499.28	Joback Method
cpl	158.70	J/mol×K	298.10	NIST Webbook
cpl	158.40	J/mol×K	298.15	NIST Webbook
cps	112.10	J/mol×K	226.10	NIST Webbook
dvisc	0.0004524	Pa×s	420.73	Joback Method
dvisc	0.0041749	Pa×s	241.86	Joback Method
dvisc	0.0003575	Pa×s	456.50	Joback Method
dvisc	0.0021288	Pa×s	277.63	Joback Method
dvisc	0.0005981	Pa×s	384.95	Joback Method
dvisc	0.0008374	Pa×s	349.18	Joback Method
dvisc	0.0012659	Pa×s	313.41	Joback Method
hfust	9.75	kJ/mol	241.80	NIST Webbook
hfust	9.75	kJ/mol	241.83	NIST Webbook
hfust	9.75	kJ/mol	241.83	NIST Webbook
hfust	9.75	kJ/mol	241.80	NIST Webbook
hvapt	41.10	kJ/mol	570.50	NIST Webbook
hvapt	43.10	kJ/mol	249.00	NIST Webbook
hvapt	39.50	kJ/mol	461.60	KDB
hvapt	40.00	kJ/mol	275.50	NIST Webbook
hvapt	51.40	kJ/mol	315.50	NIST Webbook
hvapt	46.00	kJ/mol	450.50	NIST Webbook
pvap	0.06	kPa	286.80	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.10	kPa	293.00	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.39	kPa	314.60	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.32	kPa	311.80	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.05	kPa	283.80	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.27	kPa	308.70	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.08	kPa	289.90	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.22	kPa	305.70	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.10	kPa	294.00	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.13	kPa	296.80	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.15	kPa	299.60	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.19	kPa	302.60	Thermochemistry of Halogen-Substituted Methylbenzenes
rhol	1855.00	kg/m3	277.00	KDB
sfust	40.31	J/mol×K	241.83	NIST Webbook
sfust	40.31	J/mol×K	241.83	NIST Webbook
srf	0.04	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43953e+01
Coeff. B	-3.99844e+03
Coeff. C	-5.26870e+01
Temperature range (K), min.	336.11
Temperature range (K), max.	492.86

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.00267e+01
Coeff. B	-8.12638e+03
Coeff. C	-7.90248e+00
Coeff. D	3.17808e-06
Temperature range (K), min.	241.83
Temperature range (K), max.	721.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1686.mol
Cheméo Relay (1.0):	
Enthalpies and Gibbs free energies of solvation in ethylene glycol at298 K: Influence of the solvophobic effect:	https://www.doi.org/10.1016/j.fluid.2013.06.028
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C591504&Units=SI
Examination of hydrogen-bonding interactions between dissolved solutes and alkylbenzene solvents based on Abraham model correlations derived from measured enthalpies of solvation:	https://www.doi.org/10.1016/j.tca.2014.08.024
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1686
Phase behavior of ionic liquids 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imides with fluorinated benzenes:	https://www.doi.org/10.1016/j.jct.2015.04.012
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Partitioning Coefficients of Numerous Organic Solutes between a Long-Chain Aliphatic Alcohol and the Gas Phase as a Function of Temperature:	https://www.doi.org/10.1021/je050368h
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
Cheméo Relay (1.0, beta):	
Solubilities of 4-Phenyltoluene, Phenylboric Acid, Biphenyl, and Iodobenzene in Carbon Dioxide from Measurements of the Relative Permittivity:	https://www.doi.org/10.1021/je050075o
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Liquid-Liquid Equilibria in Binary Mixtures Containing Chlorobenzene, Bromobenzene, and Iodobenzene with Ionic Liquid 1-Ethyl-3-methylimidazolim Bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1021/je801005y

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment

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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter