Benzene, 1,4-diiodo-

Other names:	1,4-Diiodbenzene
	1,4-Diiodobenzene
	Benzene, 1,4-iodo-
	Benzene, p-diiodo-
	p-Benzene diiodide
	p-Diiodobenzene
Inchi:	InChI=1S/C6H4I2/c7-5-1-2-6(8)4-3-5/h1-4H
InchiKey:	LFMWZTSOMGDDJU-UHFFFAOYSA-N
Formula:	C6H4I2
SMILES:	Ic1ccc(I)cc1
Mol. weight [g/mol]:	329.90
CAS:	624-38-4

Physical Properties

Property code	Value	Unit	Source
chs	-3093.20 ± 4.20	kJ/mol	NIST Webbook
gf	218.66	kJ/mol	Joback Method
hf	211.63	kJ/mol	Joback Method
hfus	13.76	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
ie	8.45	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-5.37		Aqueous Solubility Prediction Method
logp	2.896		Crippen Method
mcvol	123.280	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2176.00		NIST Webbook
tb	558.20	K	NIST Webbook
tc	852.28	K	Joback Method

tf	403.98	K	Aqueous Solubility Prediction Method
tf	402.15 ± 0.50	K	NIST Webbook
tf	400.00 ± 2.00	K	NIST Webbook
tf	402.00 ± 2.00	K	NIST Webbook
tf	403.15	K	Thermal, physicochemical and microstructural studies of organic analog of nonmetal-nonmetal monotectic alloy
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.55	J/mol×K	653.84	Joback Method
cpg	213.79	J/mol×K	852.28	Joback Method
cpg	209.25	J/mol×K	802.67	Joback Method
cpg	204.27	J/mol×K	753.06	Joback Method
cpg	198.74	J/mol×K	703.45	Joback Method
cpg	177.80	J/mol×K	554.62	Joback Method
cpg	185.61	J/mol×K	604.23	Joback Method
cps	160.77	J/mol×K	298.15	NIST Webbook
dvisc	0.0016788	Pa×s	352.80	Joback Method
dvisc	0.0010637	Pa×s	393.17	Joback Method
dvisc	0.0007337	Pa×s	433.53	Joback Method
dvisc	0.0005391	Pa×s	473.89	Joback Method
dvisc	0.0029814	Pa×s	312.44	Joback Method
dvisc	0.0003330	Pa×s	554.62	Joback Method
dvisc	0.0004158	Pa×s	514.26	Joback Method
hfust	22.30	kJ/mol	402.40	NIST Webbook
hfust	22.37	kJ/mol	402.00	NIST Webbook
hfust	22.37	kJ/mol	402.00	NIST Webbook
hfust	22.34	kJ/mol	402.00	NIST Webbook
hfust	22.38	kJ/mol	402.15	NIST Webbook
hsubt	63.40	kJ/mol	386.50	NIST Webbook
hvapt	52.60	kJ/mol	481.00	NIST Webbook
sfust	55.60	J/mol×K	402.15	NIST Webbook
sfust	55.60	J/mol×K	402.00	NIST Webbook
sfust	55.65	J/mol×K	402.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51398e+01
Coeff. B	-4.85971e+03
Coeff. C	-9.63160e+01
Temperature range (K), min.	423.52
Temperature range (K), max.	590.77

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624384&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
Thermal, physicochemical and microstructural studies of organic analog of nonmetal-nonmetal monotectic alloy:	https://www.doi.org/10.1016/j.tca.2009.10.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid 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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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https://www.chemeo.com/cid/70-879-9/Benzene-1-4-diiodo.pdf

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