Benzene, 1-chloro-2-iodo-

Other names:	1-Chloro-2-iodobenzene
	2-Chloroiodobenzene
	2-Chlorophenyl iodide
	2-Iodochlorobenzene
	o-Chloroiodobenzene
	o-Iodochlorobenzene
Inchi:	InChI=1S/C6H4ClI/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	MPEOPBCQHNWNFB-UHFFFAOYSA-N
Formula:	C6H4ClI
SMILES:	Clc1ccccc1I
Mol. weight [g/mol]:	238.45
CAS:	615-41-8

Physical Properties

Property code	Value	Unit	Source
gf	148.61	kJ/mol	Joback Method
hf	119.02	kJ/mol	Joback Method
hfus	13.55	kJ/mol	Joback Method
hvap	45.65	kJ/mol	Joback Method
ie	8.40 ± 0.10	eV	NIST Webbook
log10ws	-3.54		Estimated Solubility Method
log10ws	-3.54		Aqueous Solubility Prediction Method
logp	2.945		Crippen Method
mcvol	109.700	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1205.90		NIST Webbook
rinpol	1205.90		NIST Webbook
tb	507.70	K	NIST Webbook
tc	763.15	K	Joback Method
tf	274.05	K	Aqueous Solubility Prediction Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.37	J/mol×K	498.91	Joback Method
cpg	198.65	J/mol×K	719.11	Joback Method
cpg	193.04	J/mol×K	675.07	Joback Method
cpg	186.87	J/mol×K	631.03	Joback Method
cpg	180.07	J/mol×K	586.99	Joback Method
cpg	172.59	J/mol×K	542.95	Joback Method
cpg	203.75	J/mol×K	763.15	Joback Method
dvisc	0.0003439	Pa×s	498.91	Joback Method
dvisc	0.0004261	Pa×s	463.14	Joback Method
dvisc	0.0005472	Pa×s	427.37	Joback Method
dvisc	0.0007356	Pa×s	391.61	Joback Method
dvisc	0.0010494	Pa×s	355.84	Joback Method
dvisc	0.0016208	Pa×s	320.07	Joback Method
dvisc	0.0027929	Pa×s	284.30	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615418&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas 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
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume