

Benzene, 1-chloro-3-iodo-

Other names:	1-Chloro-3-iodobenzene 3-Chloro-1-iodobenzene 3-Chloriodobenzene 3-Iodochlorobenzene m-Chloriodobenzene m-Chlorophenyl iodide
Inchi:	InChI=1S/C6H4ClI/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	JMLWXCJXOYDXRN-UHFFFAOYSA-N
Formula:	C6H4ClI
SMILES:	Clc1cccc(I)c1
Mol. weight [g/mol]:	238.45
CAS:	625-99-0

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
log10ws	-3.55		Aqueous Solubility Prediction Method
log10ws	-3.55		Estimated Solubility Method
logp	2.945		Crippen Method
mcvol	109.700	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	503.20	K	NIST Webbook
tc	763.15	K	Joback Method
tf	284.30	K	Joback 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	172.59	J/mol×K	542.95	Joback Method
cpg	180.07	J/mol×K	586.99	Joback Method
cpg	186.87	J/mol×K	631.03	Joback Method
cpg	193.04	J/mol×K	675.07	Joback Method
cpg	198.65	J/mol×K	719.11	Joback Method
cpg	203.75	J/mol×K	763.15	Joback Method
dvisc	0.0027929	Pa×s	284.30	Joback Method
dvisc	0.0016208	Pa×s	320.07	Joback Method
dvisc	0.0010494	Pa×s	355.84	Joback Method
dvisc	0.0007356	Pa×s	391.61	Joback Method
dvisc	0.0005472	Pa×s	427.37	Joback Method
dvisc	0.0004261	Pa×s	463.14	Joback Method
dvisc	0.0003439	Pa×s	498.91	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.70	K	2.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
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=C625990&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/81-006-5/Benzene-1-chloro-3-iodo.pdf>

Generated by Cheméo on 2025-12-05 17:33:01.044272287 +0000 UTC m=+4704178.574312956.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.