Benzene, 1-bromo-2-iodo-

Other names:	o-Bromoiodobenzene
	1-Bromo-2-iodobenzene
	2-Bromoiodobenzene
Inchi:	InChI=1S/C6H4BrI/c7-5-3-1-2-4-6(5)8/h1-4H
InchiKey:	OIRHKGBNGGSCGS-UHFFFAOYSA-N
Formula:	C6H4BrI
SMILES:	Brc1ccccc1I
Mol. weight [g/mol]:	282.90
CAS:	583-55-1

Physical Properties

Property code	Value	Unit	Source
gf	174.86	kJ/mol	Joback Method
hf	161.09	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	47.70	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.054		Crippen Method
mcvol	114.960	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1300.00		NIST Webbook
tb	527.64	K	Joback Method
tc	804.32	K	Joback Method
tf	275.25 ± 0.50	K	NIST Webbook
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.93	J/mol×K	758.21	Joback Method
cpg	171.17	J/mol×K	527.64	Joback Method
cpg	179.16	J/mol×K	573.75	Joback Method
cpg	186.35	J/mol×K	619.87	Joback Method

cpg	192.82	J/mol×K	665.98	Joback Method
cpg	198.65	J/mol×K	712.10	Joback Method
cpg	208.72	J/mol×K	804.32	Joback Method
cpl	179.90	J/mol×K	298.15	NIST Webbook
dvisc	0.0003477	Pa×s	527.64	Joback Method
dvisc	0.0023919	Pa×s	314.18	Joback Method
dvisc	0.0014728	Pa×s	349.76	Joback Method
dvisc	0.0009918	Pa×s	385.33	Joback Method
dvisc	0.0007141	Pa×s	420.91	Joback Method
dvisc	0.0005411	Pa×s	456.49	Joback Method
dvisc	0.0004269	Pa×s	492.06	Joback Method
hfust	14.44	kJ/mol	275.25	NIST Webbook
hfust	14.42	kJ/mol	294.20	NIST Webbook
sfust	52.50	J/mol×K	275.25	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	530.20	K	101.00	NIST Webbook
tbrp	393.70	K	2.00	NIST Webbook
tbrp	393.00	K	2.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C583551&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
cpl: Liquid 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
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
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume