1-BROMO-4-IODOBENZENE

Other names:	4-Bromoiodobenzene
	p-Bromoiodobenzene
	p-Bromophenyl iodide
	p-Iodobromobenzene
Inchi:	InChI=1S/C6H4BrI/c7-5-1-3-6(8)4-2-5/h1-4H
InchiKey:	UCCUXODGPMAHRL-UHFFFAOYSA-N
Formula:	C6H4BrI
SMILES:	Brc1ccc(I)cc1
Mol. weight [g/mol]:	282.91

Physical Properties

Property code	Value	Unit	Source
af	0.3116		Cheméo Relay (1.0)
gf	174.86	kJ/mol	Joback Method
hf	193.66	kJ/mol	Cheméo Relay (1.0)
hfus	14.64	kJ/mol	Joback Method
hsub	78.50 ± 0.40	kJ/mol	NIST Webbook
hsub	78.53 ± 0.16	kJ/mol	NIST Webbook
hvap	58.08	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	NIST Webbook
log10ws	-4.56		Estimated Solubility Method
log10ws	-4.56		Aqueous Solubility Prediction Method
logp	3.054		Crippen Method
mcvol	114.960	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	519.79	K	Cheméo Relay (1.0)
tc	761.73	K	Cheméo Relay (1.0)
tf	364.48	K	Aqueous Solubility Prediction Method
tf	363.25 ± 0.50	K	NIST Webbook
vc	0.390	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	203.93	J/mol×K	758.21	Joback Method
cpg	208.72	J/mol×K	804.32	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
dvisc	0.0003477	Pa×s	527.64	Joback Method
hfust	19.38	kJ/mol	363.50	NIST Webbook
hfust	19.13	kJ/mol	363.30	NIST Webbook
hfust	19.61	kJ/mol	363.25	NIST Webbook
sfust	54.00	J/mol×K	363.25	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.20	K	1.90	NIST Webbook
tbrp	525.20	K	101.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C589877&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
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