iodine bromide

Other names: Iodine monobromide
Inchi: InChI=1S/BrI/c1-2
InchiKey: CBEQRNSPHCCXSH-UHFFFAOYSA-N
Formula: BrI
SMILES: BrI
Mol. weight [g/mol]: 206.81
CAS: 7789-33-5

Physical Properties

Property code	Value	Unit	Source
dm	1.20	debye	KDB
ea	2.51 ± 0.00	eV	NIST Webbook
ea	1.62 ± 0.05	eV	NIST Webbook
ea	2.70 ± 0.20	eV	NIST Webbook
ea	2.55 ± 0.10	eV	NIST Webbook
ea	2.55 ± 0.10	eV	NIST Webbook
gf	3.71	kJ/mol	KDB
hf	409.10	kJ/mol	KDB
hfus	5.45	kJ/mol	Joback Method
hvap	31.40	kJ/mol	Joback Method
ie	9.85	eV	NIST Webbook
ie	9.79 ± 0.00	eV	NIST Webbook
ie	9.79 ± 0.01	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
ie	9.79 ± 0.01	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	1.731		Crippen Method
mcvol	54.180	ml/mol	McGowan Method
pc	7292.66	kPa	Joback Method
tb	389.00	K	KDB
tc	719.00	K	KDB
tf	313.00	K	KDB
vc	0.139	m3/kmol	KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	38.13	J/mol×K	358.70	Joback Method
cpg	38.53	J/mol×K	398.06	Joback Method
cpg	38.77	J/mol×K	437.42	Joback Method
cpg	38.87	J/mol×K	476.78	Joback Method
cpg	38.85	J/mol×K	516.14	Joback Method
cpg	38.72	J/mol×K	555.51	Joback Method
cpg	38.53	J/mol×K	594.87	Joback Method
dvisc	0.0038740	Pa×s	207.62	Joback Method
dvisc	0.0023609	Pa×s	232.80	Joback Method
dvisc	0.0015848	Pa×s	257.98	Joback Method
dvisc	0.0011420	Pa×s	283.16	Joback Method
dvisc	0.0008682	Pa×s	308.34	Joback Method
dvisc	0.0006879	Pa×s	333.52	Joback Method
dvisc	0.0005631	Pa×s	358.70	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1896.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7789335&Units=SI

Legend

cpg: Ideal gas heat capacity
dm: Dipole Moment
dvisc: Dynamic viscosity
ea: Electron affinity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume