Benzene, 1-bromo-4-nitro-

Other names:	p-Bromonitrobenzene
	p-Nitrobromobenzene
	1-Bromo-4-nitrobenzene
	4-Bromonitrobenzene
	4-Nitrobromobenzene
Inchi:	InChI=1S/C6H4BrNO2/c7-5-1-3-6(4-2-5)8(9)10/h1-4H
InchiKey:	ZDFBKZUDCQQKAC-UHFFFAOYSA-N
Formula:	C6H4BrNO2
SMILES:	O=[N+]([O-])c1ccc(Br)cc1
Mol. weight [g/mol]:	202.00
CAS:	586-78-7

Physical Properties

Property code	Value	Unit	Source
ea	1.34 ± 0.05	eV	NIST Webbook
ea	1.29 ± 0.10	eV	NIST Webbook
gf	152.29	kJ/mol	Joback Method
hf	73.46	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hsub	86.60 ± 0.60	kJ/mol	NIST Webbook
hvap	54.91	kJ/mol	Joback Method
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-3.29		Crippen Method
logp	2.357		Crippen Method
mcvol	106.560	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	529.20	K	NIST Webbook
tc	856.92	K	Joback Method
tf	397.00 ± 205.00	K	NIST Webbook
tf	398.00 ± 2.00	K	NIST Webbook
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.37	J/mol×K	586.34	Joback Method
cpg	216.09	J/mol×K	631.44	Joback Method
cpg	223.99	J/mol×K	676.53	Joback Method
cpg	231.15	J/mol×K	721.63	Joback Method
cpg	237.63	J/mol×K	766.73	Joback Method
cpg	243.48	J/mol×K	811.83	Joback Method
cpg	248.78	J/mol×K	856.92	Joback Method
hsubt	86.60 ± 0.60	kJ/mol	299.00	NIST Webbook
hsubt	88.30	kJ/mol	298.00	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=C586787&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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