1-Bromo-2-nitrobenzene

Other names:	2-Bromo-1-nitrobenzene
	2-Bromonitrobenzene
	2-Nitrobromobenzene
	NSC 403836
	benzene, 1-bromo-2-nitro-
	o-Nitrobromobenzene
	o-Nitrophenyl bromide
	o-bromonitrobenzene
Inchi:	InChI=1S/C6H4BrNO2/c7-5-3-1-2-4-6(5)8(9)10/h1-4H
InchiKey:	ORPVVAKYSXQCJI-UHFFFAOYSA-N
Formula:	C6H4BrNO2
SMILES:	O=[N+]([O-])c1ccccc1Br
Mol. weight [g/mol]:	202.01

Physical Properties

Property code	Value	Unit	Source
ea	1.16 ± 0.10	eV	NIST Webbook
hf	94.88	kJ/mol	Cheméo Relay (1.0)
hfus	21.59	kJ/mol	Joback Method
hsub	85.20 ± 0.30	kJ/mol	NIST Webbook
hvap	65.28	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.357		Crippen Method
mcvol	106.560	ml/mol	McGowan Method
rinpol	1276.00		NIST Webbook
tb	534.20	K	NIST Webbook
tf	329.00 ± 2.00	K	NIST Webbook
tf	310.00 ± 1.50	K	NIST Webbook

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	85.50 ± 0.30	kJ/mol	285.00	NIST Webbook
psub	2.79e-04	kPa	283.17	Thermochemical study of the monobromonitrobenzene isomers
psub	3.50e-04	kPa	285.17	Thermochemical study of the monobromonitrobenzene isomers
psub	9.40e-05	kPa	275.15	Thermochemical study of the monobromonitrobenzene isomers
psub	1.24e-04	kPa	277.15	Thermochemical study of the monobromonitrobenzene isomers
psub	1.23e-04	kPa	277.15	Thermochemical study of the monobromonitrobenzene isomers
psub	1.23e-04	kPa	277.15	Thermochemical study of the monobromonitrobenzene isomers
psub	1.64e-04	kPa	279.16	Thermochemical study of the monobromonitrobenzene isomers
psub	1.65e-04	kPa	279.16	Thermochemical study of the monobromonitrobenzene isomers
psub	1.65e-04	kPa	279.16	Thermochemical study of the monobromonitrobenzene isomers
psub	2.08e-04	kPa	281.17	Thermochemical study of the monobromonitrobenzene isomers
psub	2.10e-04	kPa	281.17	Thermochemical study of the monobromonitrobenzene isomers
psub	2.12e-04	kPa	281.17	Thermochemical study of the monobromonitrobenzene isomers

psub	9.50e-05	kPa	275.15	Thermochemical study of the monobromonitrobenzene isomers
psub	2.80e-04	kPa	283.17	Thermochemical study of the monobromonitrobenzene isomers
psub	2.77e-04	kPa	283.17	Thermochemical study of the monobromonitrobenzene isomers
psub	3.51e-04	kPa	285.17	Thermochemical study of the monobromonitrobenzene isomers
psub	3.53e-04	kPa	285.17	Thermochemical study of the monobromonitrobenzene isomers
psub	9.40e-05	kPa	275.15	Thermochemical study of the monobromonitrobenzene isomers
psub	4.51e-04	kPa	287.21	Thermochemical study of the monobromonitrobenzene isomers
psub	4.59e-04	kPa	287.21	Thermochemical study of the monobromonitrobenzene isomers
psub	4.48e-04	kPa	287.21	Thermochemical study of the monobromonitrobenzene isomers
psub	5.81e-04	kPa	289.17	Thermochemical study of the monobromonitrobenzene isomers
psub	5.92e-04	kPa	289.17	Thermochemical study of the monobromonitrobenzene isomers
psub	5.94e-04	kPa	289.17	Thermochemical study of the monobromonitrobenzene isomers
psub	7.33e-04	kPa	291.14	Thermochemical study of the monobromonitrobenzene isomers
psub	7.29e-04	kPa	291.14	Thermochemical study of the monobromonitrobenzene isomers
psub	7.35e-04	kPa	291.14	Thermochemical study of the monobromonitrobenzene isomers

psub	9.13e-04	kPa	293.14	Thermochemical study of the monobromonitrobenzene isomers
psub	9.39e-04	kPa	293.14	Thermochemical study of the monobromonitrobenzene isomers
psub	9.25e-04	kPa	293.14	Thermochemical study of the monobromonitrobenzene isomers
psub	1.20e-03	kPa	295.16	Thermochemical study of the monobromonitrobenzene isomers
psub	1.21e-03	kPa	295.16	Thermochemical study of the monobromonitrobenzene isomers
psub	1.22e-03	kPa	295.16	Thermochemical study of the monobromonitrobenzene isomers

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical study of the monobromonitrobenzene isomers:	https://www.doi.org/10.1016/j.jct.2009.06.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577195&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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