

Benzene, 1-bromo-2-nitro-

Other names:	o-Bromonitrobenzene 1-Bromo-2-nitrobenzene 2-Bromonitrobenzene o-Nitrobromobenzene 2-Nitrobromobenzene o-Nitrophenyl bromide 2-Bromo-1-nitrobenzene NSC 403836
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-])c1cccc1Br
Mol. weight [g/mol]:	202.00
CAS:	577-19-5

Physical Properties

Property code	Value	Unit	Source
ea	1.16 ± 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	85.20 ± 0.30	kJ/mol	NIST Webbook
hvap	54.91	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.357		Crippen Method
mcvol	106.560	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
rinpol	1276.00		NIST Webbook
tb	534.20	K	NIST Webbook
tc	856.92	K	Joback Method
tf	329.00 ± 2.00	K	NIST Webbook
tf	310.00 ± 1.50	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	85.50 ± 0.30	kJ/mol	285.00	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=C577195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvpap:	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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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