Benzene, 1,4-dibromo-2-nitro-

Other names:	1,4-dibromo-2-nitrobenzene
	2,5-dibromonitrobenzene
Inchi:	InChI=1S/C6H3Br2NO2/c7-4-1-2-5(8)6(3-4)9(10)11/h1-3H
InchiKey:	WRGKKASJBOREMB-UHFFFAOYSA-N
Formula:	C6H3Br3NO2
SMILES:	O=[N+]([O-])c1cc(Br)ccc1Br
Mol. weight [g/mol]:	360.81
CAS:	3460-18-2

Physical Properties

Property code	Value	Unit	Source
gf	156.98	kJ/mol	Joback Method
hf	88.32	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hsub	97.00 ± 0.40	kJ/mol	NIST Webbook
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.120		Crippen Method
mcvol	124.060	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	657.48	K	Joback Method
tc	941.96	K	Joback Method
tf	472.05	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.11	J/mol×K	704.89	Joback Method
cpg	263.72	J/mol×K	941.96	Joback Method
cpg	259.35	J/mol×K	894.55	Joback Method
cpg	254.59	J/mol×K	847.14	Joback Method
cpg	249.34	J/mol×K	799.72	Joback Method
cpg	243.55	J/mol×K	752.31	Joback Method

cpg	229.96	J/mol×K	657.48	Joback Method
hsubt	96.80 ± 0.40	kJ/mol	312.00	NIST Webbook
psub	4.18e-04	kPa	314.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	2.03e-04	kPa	308.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	2.04e-04	kPa	308.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	2.05e-04	kPa	308.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	2.60e-04	kPa	310.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	2.64e-04	kPa	310.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers

psub	2.61e-04	kPa	310.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	3.27e-04	kPa	312.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	3.32e-04	kPa	312.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	3.29e-04	kPa	312.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	4.18e-04	kPa	314.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	4.19e-04	kPa	314.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.63e-04	kPa	306.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers

psub	5.22e-04	kPa	316.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	5.27e-04	kPa	316.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	5.24e-04	kPa	316.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	6.66e-04	kPa	318.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	6.75e-04	kPa	318.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	6.73e-04	kPa	318.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	8.84e-04	kPa	320.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers

psub	8.58e-04	kPa	320.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	8.38e-04	kPa	320.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.07e-03	kPa	322.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.07e-03	kPa	322.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.06e-03	kPa	322.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.66e-04	kPa	306.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.67e-04	kPa	306.15	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers

psub	1.23e-04	kPa	304.16	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.25e-04	kPa	304.16	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	1.21e-04	kPa	304.16	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	9.70e-05	kPa	302.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	9.70e-05	kPa	302.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers
psub	9.90e-05	kPa	302.14	Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3460182&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study of the 2,5-dibromonitrobenzene isomer: An approach of the energetic study for the other dibromonitrobenzene isomers:	https://www.doi.org/10.1016/j.jct.2009.05.010
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
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume