Borazine

Other names:	1,3,5,2,4,6-Triazatriborine, hexahydro-
	B3H6N3
	Borazole
	Borazyne, cyclic trimer
	Hexahydro-s-triazaborine
	Triborinetriamine
	s-Triazatriborine, hexahydro-
Inchi:	InChI=1S/B3H6N3/c1-4-2-6-3-5-1/h1-6H
InchiKey:	BGECDVWSWDRFSP-UHFFFAOYSA-N
Formula:	B3H6N3
SMILES:	B1NBNBN1
Mol. weight [g/mol]:	80.50
CAS:	6569-51-3

Physical Properties

Property code	Value	Unit	Source
affp	802.50	kJ/mol	NIST Webbook
basg	772.80	kJ/mol	NIST Webbook
ie	9.88	eV	NIST Webbook
ie	10.14 ± 0.01	eV	NIST Webbook
ie	9.88 ± 0.02	eV	NIST Webbook
ie	10.01 ± 0.01	eV	NIST Webbook
ie	9.77	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
logp	-3.432		Crippen Method
tt	215.76 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	10.61	kJ/mol	161.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45538e+01
Coeff. B	-2.88879e+03
Coeff. C	-3.53900e+01
Temperature range (K), min.	210.15
Temperature range (K), max.	326.15

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6569513&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
hfust: Enthalpy of fusion at a given temperature
ie: Ionization energy
logp: Octanol/Water partition coefficient
pvap: Vapor pressure
tt: Triple Point Temperature