

s-Triazaborane

Other names:	1,3,5,2,4,6-Triazatriborine, hexahydro-B3H6N3 Borazine 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
log10ws	7.37		Crippen Method
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	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6569513&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure
tt:	Triple Point Temperature

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