Borane, triethyl-

Other names:	Triethylborane
	Triethylboron
	(C2H5)3B
	Triethylborine
	Borethyl
Inchi:	InChI=1S/C6H15B/c1-4-7(5-2)6-3/h4-6H2,1-3H3
InchiKey:	LALRXNPLTWZJIJ-UHFFFAOYSA-N
Formula:	C6H15B
SMILES:	CCB(CC)CC
Mol. weight [g/mol]:	97.99
CAS:	97-94-9

Physical Properties

Property code	Value	Unit	Source
ie	9.60	eV	NIST Webbook
ie	9.70 ± 0.10	eV	NIST Webbook
ie	9.00 ± 0.20	eV	NIST Webbook
log10ws	0.16		Crippen Method
logp	2.541		Crippen Method
ss	330.05	J/mol×K	NIST Webbook
ss	338.10	J/mol×K	NIST Webbook
tb	321.81	K	NIST Webbook
tt	180.21 ± 0.05	K	NIST Webbook
tt	180.30 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	240.00	J/mol×K	298.15	NIST Webbook
cps	241.40	J/mol×K	300.00	NIST Webbook
hfust	11.52	kJ/mol	180.21	NIST Webbook
hfust	11.85	kJ/mol	180.30	NIST Webbook
hfust	11.85	kJ/mol	180.30	NIST Webbook
hvapt	3.67	kJ/mol	300.00	NIST Webbook

hvapt	33.60	kJ/mol	293.00	NIST Webbook
sfust	63.94	J/mol×K	180.21	NIST Webbook
svapt	122.00	J/mol×K	300.00	NIST Webbook

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=C97949&Units=SI

Legend

cps: Solid phase heat capacity

hfust: Enthalpy of fusion at a given temperature

hvapt: Enthalpy of vaporization at a given temperature

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

sfust: Entropy of fusion at a given temperature

ss: Solid phase molar entropy at standard conditions

svapt: Entropy of vaporization at a given temperature

tb: Normal Boiling Point Temperature

tt: Triple Point Temperature