2,8,9-TRIOXA-5-AZA-1-BORABICYCLO[3.3.3]UND

Other names:	Boratran
	Boratrane
	Boric acid, tris(2-aminoethyl) ester
	Boron, ((2,2',2''-nitrilotris(ethanolato))(3-))-
	Ethanol, 2,2',2''-nitrilotri-, cyclic ester with boric acid (H3BO3) (1:1)
	Ethanol, 2,2',2''-nitrilotris-, cyclic ester with boric acid (H3BO3) (1:1)
	Triethanolamine borate
	Atracor T
	Ethanol, 2,2',2''-nitrilotri-, cyclic borate
	NSC 5220
Inchi:	InChI=1S/C6H12BNO3/c1-4-9-7-10-5-2-8(1)3-6-11-7/h1-6H2
InchiKey:	NKPKVNRBHXOADG-UHFFFAOYSA-N
Formula:	C6H12BNO3
SMILES:	C1CN2CCOB(O1)OCC2
Mol. weight [g/mol]:	156.98

Physical Properties

Property code	Value	Unit	Source
ie	9.80	eV	NIST Webbook
logp	-0.650		Crippen Method
ss	183.20	J/mol×K	NIST Webbook
ss	216.20	J/mol×K	NIST Webbook
tt	499.40 ± 1.50	K	NIST Webbook
tt	511.86 ± 0.01	K	NIST Webbook
tt	511.86 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	187.20	J/mol×K	298.15	NIST Webbook
cps	226.40	J/mol×K	320.00	NIST Webbook
hfust	8.78	kJ/mol	499.40	NIST Webbook
hsubt	111.90 ± 0.90	kJ/mol	418.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C283567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cps:	Solid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
ss:	Solid phase molar entropy at standard conditions
tt:	Triple Point Temperature