Borane carbonyl

Other names:	BH3CO
	Borane, compd. with carbon monoxide (1:1)
	Borane-carbon monoxide (1:1)
	Borine carbonyl (BH3CO)
	Boron, carbonyltrihydro-
	Boron, carbonyltrihydro-, (T-4)-
	Carbon monoxide-borane
Inchi:	InChI=1S/CH3BO/c2-1-3/h2H3
InchiKey:	ZJUVLBOEAXFSHP-UHFFFAOYSA-N
Formula:	CH3BO
SMILES:	[BH3-]C#[O+]
Mol. weight [g/mol]:	41.84
CAS:	13205-44-2

Physical Properties

Property code	Value	Unit	Source
ie	11.14 ± 0.02	eV	NIST Webbook
ie	11.92 ± 0.02	eV	NIST Webbook
log10ws	-1.42		Crippen Method
logp	-1.301		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	19.70	kJ/mol	171.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(Pvp) = A + B/(T + C)$

Coeff. A	1.64002e+01
Coeff. B	-2.51030e+03
Coeff. C	3.91400e+00
Temperature range (K), min.	149.15
Temperature range (K), max.	222.47

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C13205442&Units=SI

Legend

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pvap:	Vapor pressure