

Borane-methyl sulfide complex

Other names:	Borane dimethylsulfide complex Borane, compd. with dimethylsulfide Borane-dimethylsulfide Boron, trihydro[thiobis[methane]]-, (T-4)- Dimethyl sulfide borane Dimethyl sulfide-borane complex Methyl sulfide, compd. with borane (1:1) dimethyl sulphide--borane
Inchi:	InChI=1S/C2H9BS/c1-4(2)3/h1-3H3
InchiKey:	IRTZFNXVGJHNHS-UHFFFAOYSA-N
Formula:	C2H6S.BH3
SMILES:	[BH2-][S+](C)C
Mol. weight [g/mol]:	75.97
CAS:	13292-87-0

Physical Properties

Property code	Value	Unit	Source
log10ws	3.70		Crippen Method
logp	-0.588		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	44.90	kJ/mol	293.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.16508e+01

Coeff. B	-5.40186e+03
Temperature range (K), min.	252.86
Temperature range (K), max.	330.60

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13292870&Units=SI
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

Legend

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

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