

Thioboric acid (H3BS3), trimethyl ester

Other names:	Tris(methylthio)borane
	Thioboric acid (H3BS3), trimethyl ester
	Borane, tris(methylthio)-
	Methyl thioborate, (MeS)3B
	Thioboric acid, trimethyl ester
	Trithioboric acid trimethyl ester
	B(SCH3)3
	Tris(methylsulfanyl)borane
	Trimethyl trithioborate
Inchi:	InChI=1S/C3H9BS3/c1-5-4(6-2)7-3/h1-3H3
InchiKey:	PCFXNRZVDPDCHY-UHFFFAOYSA-N
Formula:	C3H9BS3
SMILES:	CSB(SC)SC
Mol. weight [g/mol]:	152.12

Physical Properties

Property code	Value	Unit	Source
hvap	54.00 ± 0.80	kJ/mol	NIST Webbook
ie	9.24	eV	NIST Webbook
ie	8.74	eV	NIST Webbook
logp	2.060		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	44.90	kJ/mol	393.50	NIST Webbook
hvapt	51.60	kJ/mol	398.00	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C997499&Units=SI>

Legend

h_{vap}: Enthalpy of vaporization at standard conditions
h_{vapt}: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log_p: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/18-644-7/Thioboric-acid-H3BS3-trimethyl-ester.pdf>

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