Boric acid (H3BO3), tris(1-methylethyl) ester

Other names:	Boric acid (H3BO3), triisopropyl ester
	Boric acid triisopropyl ester
	Boric acid, tris(1-methylethyl) ester
	Boron isopropoxide
	Boron triisopropoxide
	Isopropyl borate
	Isopropyl borate, ((C3H7O)3B)
	NSC 9779
	Triisopropoxyborane
	Triisopropoxyboron
	Triisopropyl borate
	Triisopropyl orthoborate
	UN 2616
	tri-i-Propylborate
Inchi:	InChI=1S/C9H21BO3/c1-7(2)11-10(12-8(3)4)13-9(5)6/h7-9H,1-6H3
InchiKey:	NHDIQVFFNDKAQU-UHFFFAOYSA-N
Formula:	C9H21BO3
SMILES:	CC(C)OB(OC(C)C)OC(C)C
Mol. weight [g/mol]:	188.07
CAS:	5419-55-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.44		Crippen Method
logp	2.246		Crippen Method
tb	413.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	42.40	kJ/mol	375.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46655e+01
Coeff. B	-3.58829e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	305.58
Temperature range (K), max.	439.61

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5419556&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
tb:	Normal Boiling Point Temperature

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