

Boric acid, tris(2-methylpropyl) ester

Other names:	Boric acid (H ₃ BO ₃), triisobutyl ester Triisobutyl borate tri- <i>i</i> -Butylborate Boric acid, triisobutyl ester Isobutyl borate, (C ₄ H ₉ O) ₃ B
Inchi:	InChI=1S/C12H27BO3/c1-10(2)7-14-13(15-8-11(3)4)16-9-12(5)6/h10-12H,7-9H2,1-6H3
InchiKey:	LHJSLDBKUGXPMI-UHFFFAOYSA-N
Formula:	C ₁₂ H ₂₇ BO ₃
SMILES:	CC(C)COB(OCC(C)C)OCC(C)C
Mol. weight [g/mol]:	230.15
CAS:	13195-76-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.63		Crippen Method
logp	2.989		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	51.70	kJ/mol	422.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13195761&Units=SI

Legend

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

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