Boric acid, trihexyl ester

Other names:	Hexyl orthoborate
	Trihexyl borate
	Hexyl borate, tri-
	Tri-n-hexyl borate
Inchi:	InChI=1S/C18H39BO3/c1-4-7-10-13-16-20-19(21-17-14-11-8-5-2)22-18-15-12-9-6-3/h4-1
InchiKey:	KDQYHGMMZKMQAA-UHFFFAOYSA-N
Formula:	C18H39BO3
SMILES:	CCCCCCOB(OCCCCCC)OCCCCCC
Mol. weight [g/mol]:	314.31
CAS:	5337-36-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	5.762		Crippen Method

Sources

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=C5337360&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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