

Tripropyl borate

Other names:	Boric acid (H3BO3), tripropyl ester
	Boric acid, tripropyl ester
	Boron propoxide
	Propyl orthoborate
	Tripropoxyborane
	Tripropyl orthoborate
	Tris(propoxy)borane
	(n-C3H7O)3B
	tri-n-Propyl borate
	Boric acid tri-n-propyl ester
	Propyl borate, (PrO)3B
	NSC 778
Inchi:	InChI=1S/C9H21BO3/c1-4-7-11-10(12-8-5-2)13-9-6-3/h4-9H2,1-3H3
InchiKey:	LTEHWCCSIHAVOQ-UHFFFAOYSA-N
Formula:	C9H21BO3
SMILES:	CCCOB(OCCC)OCCC
Mol. weight [g/mol]:	188.07
CAS:	688-71-1

Physical Properties

Property code	Value	Unit	Source
ie	10.02	eV	NIST Webbook
ie	10.62 ± 0.15	eV	NIST Webbook
log10ws	-0.10		Crippen Method
logp	2.251		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	52.30	kJ/mol	396.50	NIST Webbook
hvapt	47.60	kJ/mol	405.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C688711&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/40-356-2/Tripropyl-borate.pdf>

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