

Boric acid (H3BO3), tripropyl ester

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:	LTEHWCSSIHAVOQ-UHFFFAOYSA-N
Formula:	C9H21BO3
SMILES:	CCCOB(OCCC)OCCC
Mol. weight [g/mol]:	188.08

Physical Properties

Property code	Value	Unit	Source
af	0.6381		Cheméo Relay (1.0)
gf	-352.79	kJ/mol	Cheméo Relay (1.0, beta)
hf	-811.17	kJ/mol	Cheméo Relay (1.0)
hvap	46.49	kJ/mol	Cheméo Relay (1.0)
ie	10.62 ± 0.15	eV	NIST Webbook
ie	10.02	eV	NIST Webbook
log10ws	-2.68		Cheméo Relay (1.0)
logp	2.251		Crippen Method
pc	2173.52	kPa	Cheméo Relay (1.0, beta)
tb	443.80	K	Cheméo Relay (1.0)
tc	608.25	K	Cheméo Relay (1.0)
tf	177.30	K	Cheméo Relay (1.0)
vc	0.661	m3/kmol	Cheméo Relay (1.0)

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:	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=C688711&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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