Borazine, 2,4,6-trimethyl-

Other names: B,B,B-Trimethylborazine
Inchi: InChI=1S/C3H12B3N3/c1-4-7-5(2)9-6(3)8-4/h7-9H,1-3H3
InchiKey: DXFJPBGUYITLMJ-UHFFFAOYSA-N
Formula: C3H12B3N3
SMILES: CB1NB(C)NB(C)N1
Mol. weight [g/mol]: 122.58
CAS: 5314-85-2

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.64 ± 0.03	eV	NIST Webbook
log10ws	5.46		Crippen Method
logp	-0.877		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=C5314852&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.