

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

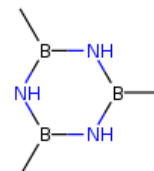
InChI Key: DXFJPBGUYITLMJ-UHFFFAOYSA-N

Formula: C3H12B3N3

SMILES: CB1NB(C)NB(C)N1

Molecular Weight: 122.58

CAS: 5314-85-2



Physical Properties

Property	Value	Unit	Source
IE	9.30	eV	NIST Webbook
IE	9.50	eV	NIST Webbook
IE	9.64 ± 0.03	eV	NIST Webbook
$\log P_{\text{oct/wat}}$	-0.88		Crippen Method

Sources

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C3H12B3N3/c1-4-7-5\(2\)9-6\(3\)8-4/h7-9H,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C3H12B3N3/c1-4-7-5(2)9-6(3)8-4/h7-9H,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

IE: Ionization energy (eV).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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