BORAZINE, HEXAMETHYL-

Inchi: InChI=1S/C6H18B3N3/c1-7-10(4)8(2)12(6)9(3)11(7)5/h1-6H3
InchiKey: LCHQMXUQYONIOI-UHFFFAOYSA-N
Formula: C6H18B3N3
SMILES: CB1N(C)B(C)N(C)B(C)N1C
Mol. weight [g/mol]: 164.67

Physical Properties

Property code	Value	Unit	Source
ie	8.77	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
logp	0.149		Crippen Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C877076&Units=SI
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):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient