

1-Aza-5-boratricyclo[3.3.3.01,5]undecane

Other names:	1-Aza-5-boratricyclo[3.3.3.0
Inchi:	InChI=1S/C9H18BN/c1-4-10-5-2-8-11(10,7-1)9-3-6-10/h1-9H2
InchiKey:	ACLOQPYOCRBNL-UHFFFAOYSA-N
Formula:	C9H18BN
SMILES:	C1C[B-]23CCC[N+]2(C1)CCC3
Mol. weight [g/mol]:	151.06
CAS:	826-15-3

Physical Properties

Property code	Value	Unit	Source
ie	8.20	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	1.15		Crippen Method
logp	1.960		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C826153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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/34-969-9/1-Aza-5-boratricyclo-3-3-3-01-5-undecane.pdf>

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