

[1,2]Azaborino[1,2-a][1,2]azaborine

Other names:	10,9-Borazaronaphthalene 4a-Azonia-8a-boratanaphthalene
Inchi:	InChI=1S/C8H8BN/c1-3-7-10-8-4-2-6-9(10)5-1/h1-8H
InchiKey:	GSVAFVMURLKGLG-UHFFFAOYSA-N
Formula:	C8H8BN
SMILES:	C1=CB2C=CC=CN2C=C1
Mol. weight [g/mol]:	128.97
CAS:	1425-58-7

Physical Properties

Property code	Value	Unit	Source
ie	8.24	eV	NIST Webbook
log10ws	-0.19		Crippen Method
logp	1.525		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1425587&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/51-578-4/1-2-Azaborino-1-2-a-1-2-azaborine.pdf>

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