

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

Other names:	Octahydro[1,2]azaborinino[1,2-a][1,2]azaborine 9-Aza-10-boradecalin
Inchi:	InChI=1S/C8H16BN/c1-3-7-10-8-4-2-6-9(10)5-1/h1-8H2
InchiKey:	VBTBGTSTOFJXPD-UHFFFAOYSA-N
Formula:	C8H16BN
SMILES:	C1CCN2CCCCB2C1
Mol. weight [g/mol]:	137.03
CAS:	18903-54-3

Physical Properties

Property code	Value	Unit	Source
ie	8.47	eV	NIST Webbook
log10ws	0.38		Crippen Method
logp	1.867		Crippen Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.50 ± 1.50	K	3.60	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18903543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
tbrp: Boiling point at reduced pressure

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