

3-Methyl-2,8,9-trioxa-5-azonia-1-boratatricyclo[3.3.3.0(1,5)]undecane

Other names:	3-Methyl-2,8,9-trioxa-5-aza-1-boratatricyclo[3.3.3.0(1,5)]undecane
Inchi:	InChI=1S/C7H14BNO3/c1-7-6-9-2-4-10-8(9,12-7)11-5-3-9/h7H,2-6H2,1H3
InchiKey:	AFOKVYQKMHSYDH-UHFFFAOYSA-N
Formula:	C7H14BNO3
SMILES:	CC1C[N+]23CCO[B-]2(OCC3)O1
Mol. weight [g/mol]:	171.00
CAS:	27664-61-5

Physical Properties

Property code	Value	Unit	Source
ie	8.90	eV	NIST Webbook
ie	9.70	eV	NIST Webbook
log10ws	2.87		Crippen Method
logp	-0.282		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27664615&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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