

2,10,11-Trioxa-6-azonia-1-boratatricyclo(4.4.3.0(1,

Other names:	2,10,11-Trioxa-5-aza-1-boratatricyclo[4.4.3.01,6]tridecane
Inchi:	InChI=1S/C8H16BNO3/c1-3-10-4-2-7-12-9(10,11-6-1)13-8-5-10/h1-8H2
InchiKey:	DVGDIZINSCCOLT-UHFFFAOYSA-N
Formula:	C8H16BNO3
SMILES:	C1CO[B-]23OCCC[N+]2(C1)CCO3
Mol. weight [g/mol]:	185.03
CAS:	283-64-7

Physical Properties

Property code	Value	Unit	Source
log10ws	2.56		Crippen Method
logp	0.110		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	102.20 ± 1.00	kJ/mol	390.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C283647&Units=SI

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

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