

2,8,9-Trioxa-5-aza-1-silabicyclo[3.3.3]undecane,

Other names:

1-ethenyl-

1-Vinylsilatrane

Vinylsilatrane

2,8,9-Trioxa-5-aza-1-silabicyclo(3.3.3)undecane, 1-vinyl-

Vinylsilatran

1-Vinyl-2,8,9-trioxa-5-aza-1-silabicyclo(3.3.3)undecane

Inchi: InChI=1S/C8H15NO3Si/c1-2-13-10-6-3-9(4-7-11-13)5-8-12-13/h2H,1,3-8H2

InchiKey: JETUZEFWCTPQD-UHFFFAOYSA-N

Formula: C8H15NO3Si

SMILES: C=C[Si]12OCCN(CCO1)CCO2

Mol. weight [g/mol]: 201.30

CAS: 2097-18-9

Physical Properties

Property code	Value	Unit	Source
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	2.05		Crippen Method
logp	0.030		Crippen Method
rinpol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	2580.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2097189&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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