

1-Ethoxysilatrane

Other names:	1-ethoxy-2,8,9-trioxa-5-aza-1-silabicyclo[3.3.3]undecane Ethoxysilatrane
Inchi:	InChI=1S/C8H17NO4Si/c1-2-10-14-9(3-6-11-14,4-7-12-14)5-8-13-14/h2-8H2,1H3
InchiKey:	AZNKYARPJPBPDW-UHFFFAOYSA-N
Formula:	C8H17NO4Si
SMILES:	CCO[Si]123OCC[N+]1(CCO2)CCO3
Mol. weight [g/mol]:	219.31
CAS:	3463-21-6

Physical Properties

Property code	Value	Unit	Source
ie	10.60	eV	NIST Webbook
log10ws	2.93		Crippen Method
logp	-0.183		Crippen Method
rinpol	1614.00		NIST Webbook
ripol	2808.00		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=C3463216&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/55-965-0/1-Ethoxysilatrane.pdf>

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