

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

Other names:

1-Methoxysilatrane
1-Methoxy-2,8,9-trioxa-5-aza-1-silabicyclo(3.3.3)undecane
Silatrane, methoxy-

Inchi: InChI=1S/C7H15NO4Si/c1-9-13-10-5-2-8(3-6-11-13)4-7-12-13/h2-7H2,1H3
InchiKey: JHUCBAOHJYDAIC-UHFFFAOYSA-N
Formula: C7H15NO4Si
SMILES: CO[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]: 205.28
CAS: 4025-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	2.74		Crippen Method
logp	-0.553		Crippen Method
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
ripol	2883.00		NIST Webbook
ripol	2883.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4025803&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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<https://www.cheméo.com/cid/21-343-7/2-8-9-Trioxa-5-aza-1-silabicyclo-3-3-3-undecane-1-methoxy.pdf>

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