

1-(«alpha»-naphthyl)silatrane

Inchi: InChI=1S/C16H19NO3Si/c1-2-6-15-14(4-1)5-3-7-16(15)21-18-11-8-17(9-12-19-21)10-13
InchiKey: GJMBSQWDMIGUJH-UHFFFAOYSA-N
Formula: C16H19NO3Si
SMILES: c1ccc2c([Si]34OCCN(CCO3)CCO4)cccc2c1
Mol. weight [g/mol]: 301.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	1.365		Crippen Method
rinpol	2718.00		NIST Webbook
rinpol	2718.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R145496&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/124-954-5/1-alpha-naphthyl-silatrane.pdf>

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