

1-benzyl, 4,4,7,10-tetramethylsilatrane, a

Inchi: InChI=1S/C17H27NO3Si/c1-14-10-18-11-15(2)21-22(20-14,19-13-17(18,3)4)12-16-8-6-5
InchiKey: QKTHTNVMCPWGHU-UHFFFAOYSA-N
Formula: C17H27NO3Si
SMILES: CC1CN2CC(C)O[Si](Cc3ccccc3)(OCC2(C)C)O1
Mol. weight [g/mol]: 321.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	2.642		Crippen Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		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=R145510&Units=SI>

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/115-157-0/1-benzyl-4-4-7-10-tetramethylsilatrane-a.pdf>

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