

1-(2-isopropyl-5-methoxyphenoxy)-silatrane

Inchi: InChI=1S/C16H25NO4Si/c1-13(2)15-12-14(3)4-5-16(15)21-22-18-9-6-17(7-10-19-22)8-1
InchiKey: ILDJHWBDEHUQGP-UHFFFAOYSA-N
Formula: C16H25NO4Si
SMILES: Cc1ccc(O[Si]23OCCN(CCO2)CCO3)c(C(C)C)c1
Mol. weight [g/mol]: 323.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.76		Crippen Method
logp	2.312		Crippen Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R145401&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/116-967-0/1-2-isopropyl-5-methoxyphenoxy-silatrane.pdf>

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