

1-(o-chlorophenyl)-silatrane

Inchi: InChI=1S/C12H16ClNO3Si/c13-11-3-1-2-4-12(11)18-15-8-5-14(6-9-16-18)7-10-17-18/h1
InchiKey: XKLVDAGNHGKDPR-UHFFFAOYSA-N
Formula: C12H16ClNO3Si
SMILES: Clc1ccccc1[Si]12OCCN(CCO1)CCO2
Mol. weight [g/mol]: 285.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	0.865		Crippen Method
rinpol	2267.00		NIST Webbook
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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=R145812&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/112-819-8/1-o-chlorophenyl-silatrane.pdf>

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