

1-(p-bromophenyl), 4,4,7,10-tetramethylsilatrane, b

Inchi: InChI=1S/C16H24BrNO3Si/c1-12-9-18-10-13(2)21-22(20-12,19-11-16(18,3)4)15-7-5-14(
InchiKey: PMFOYNXTGGJBOH-UHFFFAOYSA-N
Formula: C16H24BrNO3Si
SMILES: CC1CN2CC(C)O[Si](c3ccc(Br)cc3)(OCC2(C)C)O1
Mol. weight [g/mol]: 386.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.94		Crippen Method
logp	2.530		Crippen Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R145847&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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.chemeo.com/cid/124-280-3/1-p-bromophenyl-4-4-7-10-tetramethylsilatrane-b.pdf>

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