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

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	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R145832&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/119-020-7/1-p-bromophenyl-4-4-7-10-tetramethylsilatrane-a.pdf
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