

3,4-Dihydroxyphenylglycol, O-TMS

Inchi: InChI=1S/C17H34O4Si3/c1-22(2,3)19-13-12-18-15-10-11-16(20-23(4,5)6)17(14-15)21-22
InchiKey: GNSMEKUGGFREMJ-UHFFFAOYSA-N
Formula: C17H34O4Si3
SMILES: C[Si](C)(C)OCCOc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 386.71

Physical Properties

Property code	Value	Unit	Source
log10ws	1.58		Crippen Method
logp	5.344		Crippen Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R139149&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

Latest version available from:

<https://www.cheméo.com/cid/122-664-9/3-4-Dihydroxyphenylglycol-O-TMS.pdf>

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