

1-(4-Chlorophenyl)-4,4-dimethyl-3-(1,2,4-triazol-1-yl)trimethylsilyl ether

Other names: 1-(4-Chlorophenyl)-4,4-dimethyl-3-(1H-1,2,4-triazol-1-ylmethyl)-3-pentanol, TMS ether

Inchi: «alpha»-(2-(4-Chlorophenyl)ethyl)-«alpha»-(1,1-dimethylethyl)-1H-1,2,4-triazole-1-ethanol, TMS ether

InchiKey: NPTSCAQIVNWXHW-UHFFFAOYSA-N

Formula: C₁₉H₃₀ClN₃O_{Si}

SMILES: CC(C)(C)C(CCC1ccc(Cl)cc1)(Cn1cncn1)O[Si](C)(C)C

Mol. weight [g/mol]: 380.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	5.201		Crippen Method
rinpol	2487.00		NIST Webbook
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Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U373457&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

Latest version available from:

<https://www.chemeo.com/cid/64-045-1/1-4-Chlorophenyl-4-4-dimethyl-3-1-2-4-triazol-1-ylmethyl-pentan-3-ol-trimethylsilyl-ether>

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