

1-(2,4-Dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-5-yl)pentan-3-yltrimethylsilanyl ether

Other names:

1-(2,4-Dichlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-5-yl)pentan-3-yltrimethylsilanyl ether

InChI: InChI=1S/C18H25Cl2N3OSi/c1-18(2,3)17(24-25(4,5)6)16(23-12-21-11-22-23)10-13-7-8-

InchiKey: AVBKYZIXGYUAAJ-MHWRWJLKSA-N

Formula: C18H25Cl2N3OSi

SMILES: CC(C)(C)C(O[Si](C)(C)C)C(=Cc1ccc(Cl)c(Cl)c1)n1cncn1

Mol. weight [g/mol]: 398.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	5.849		Crippen Method
rinpol	2377.00		NIST Webbook

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=U373095&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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