

2-(2,4-Dichlorophenyl)-1-(1,2,4-triazol-1-yl)hexan-2-ol, trimethylsilyl ether

Other names: 1-Butyl-1-(2,4-dichlorophenyl)-1H-1,2,4-triazole-1-ethanol, trimethylsilyl ether
1H-1,2,4-Triazole-1-ethanol, «alpha»-butyl-«alpha»-(2,4-dichlorophenyl)-, trimethylsilyl ether
2-(2,4-Dichlorophenyl)-1-(1H-1,2,4-triazol-1-yl)-2-hexanol, trimethylsilyl ether

Inchi: InChI=1S/C17H25Cl2N3OSi/c1-5-6-9-17(23-24(2,3)4,11-22-13-20-12-21-22)15-8-7-14(16,17)/q1

InchiKey: PVJPOTGIAFHNSU-UHFFFAOYSA-N

Formula: C17H25Cl2N3OSi

SMILES: CCCCC(Cn1cncn1)(O[Si](C)(C)C)c1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 386.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	5.522		Crippen Method
rinpol	2302.00		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=U373138&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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<https://www.chemeo.com/cid/31-960-1/2-2-4-Dichlorophenyl-1-1-2-4-triazol-1-yl-hexan-2-ol-trimethylsilyl-ether.pdf>

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