

1,2-Propanediol, 3-(4-chlorophenoxy), DTBS

Inchi:	InChI=1S/C16H25ClO3Si/c1-15(2,3)21(16(4,5)6)18-11-14(20-21)19-13-9-7-12(17)8-10-1
InchiKey:	DIMCNIKGJLRNST-UHFFFAOYSA-N
Formula:	C16H25ClO3Si
SMILES:	CC(C)(C)[Si]1(C(C)(C)C)OCC(Oc2ccc(Cl)cc2)O1
Mol. weight [g/mol]:	328.91

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	5.134		Crippen Method
rinpol	2110.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41061&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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