

trans-Diethylstilbestrol diTMS

Other names:	trans-Diethylstilbestrol, bis-TMS ether trans-Diethylstilbestrol, TMS [4-((1E)-1-Ethyl-2-(4-[(trimethylsilyl)oxy]phenyl)-1-butenyl)phenoxy](trimethyl)silane
Inchi:	InChI=1S/C24H36O2Si2/c1-9-23(19-11-15-21(16-12-19)25-27(3,4)5)24(10-2)20-13-17-2
InchiKey:	XLHDQZMLRVWJCX-WCWDXBQESA-N
Formula:	C24H36O2Si2
SMILES:	CCC(=C(CC)c1ccc(O[Si](C)(C)C)cc1)c1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	412.71
CAS:	66983-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	7.845		Crippen Method
rinpol	2389.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66983877&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/32-267-0/trans-Diethylstilbestrol-diTMS.pdf>

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