1,2-Dodecanediol, DTBS

Inchi:	InChI=1S/C20H42O2Si/c1-8-9-10-11-12-13-14-15-16-18-17-21-23(22-18,19(2,3)4)20(5,6
InchiKey:	JMOBCXSEIOKGFO-UHFFFAOYSA-N
Formula:	C20H42O2Si
SMILES:	CCCCCCCCCCC1CO[Si](C(C)(C)C)(C(C)(C)C)O1
Mol. weight [g/mol]:	342.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	6.975		Crippen Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R115227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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