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

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=R115227&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices