Panaxydol, TMS

Inchi:	InChI=1S/C20H32O2Si/c1-6-8-9-10-13-16-19-20(21-19)17-14-11-12-15-18(7-2)22-23(3,4
InchiKey:	ALSRNWWLYNJWOP-UHFFFAOYSA-N
Formula:	C20H32O2Si
SMILES:	C=CC(C#CC#CCC1OC1CCCCCCC)O[Si](C)(C)C
Mol. weight [g/mol]:	332.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.09		Crippen Method
logp	4.917		Crippen Method
rinpol	2218.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414698&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

Latest version available from:

https://www.chemeo.com/cid/87-630-6/Panaxydol-TMS.pdf

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