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

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=U414698&Units=SI

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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