trans-Phenanthrene, 9,10-dihydro-9,10-diol, bis-TMS

Inchi: InChI=1S/C20H28O2Si2/c1-23(2,3)21-19-17-13-9-7-11-15(17)16-12-8-10-14-18(16)20(1

InchiKey: FWRIIENWHSRMHD-WOJBJXKFSA-N

Formula: C20H28O2Si2

SMILES: C[Si](C)(C)OC1c2ccccc2-c2ccccc2C1O[Si](C)(C)C

Mol. weight [g/mol]: 356.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	6.152		Crippen Method
rinpol	2020.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109856&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