

cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, bis-TMS

Inchi: InChI=1S/C21H30O2Si2/c1-21(23-25(5,6)7)19-15-11-10-13-17(19)16-12-8-9-14-18(16)2
InchiKey: PPOJRWZVMGHQCJ-RTWAWAEB SA-N
Formula: C₂₁H₃₀O₂Si₂
SMILES: CC1(O[Si](C)(C)C)c2ccccc2-c2ccccc2C1O[Si](C)(C)C
Mol. weight [g/mol]: 370.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	6.326		Crippen Method
rinpol	2020.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109569&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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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