

cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3-methoxy,

bis-TMS

InChI: InChI=1S/C22H32O3Si2/c1-22(25-27(6,7)8)20-12-10-9-11-17(20)19-15-16(23-2)13-14-1

InChIKey: LDTZIPSINLWFKS-YADHBBJMSA-N

Formula: C22H32O3Si2

SMILES: COc1ccc2c(c1)-c1cccc1C(C)(O[Si](C)(C)C)C2O[Si](C)(C)C

Mol. weight [g/mol]: 400.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	6.335		Crippen Method
rinpol	2360.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109529&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/19-685-1/cis-Phenanthrene-9-10-dihydro-9-methyl-9-10-diol-3-methoxy-bis-TMS.pdf>

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