Benzo[a]pyrene, trans-11,12-diol, TMS

Inchi: InChI=1S/C26H28O2Si2/c1-29(2,3)27-25-21-13-9-11-17-14-15-19-16-18-10-7-8-12-20(1
InchiKey: SEIOHUOFEVNVJT-UHFFFAOYSA-N
Formula: C26H28O2Si2
SMILES: C[Si](C)(C)Oc1c(O[Si](C)(C)C)c2c3ccccc3cc3ccc4cccc1c4c32
Mol. weight [g/mol]: 428.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.12		Crippen Method
logp	8.165		Crippen Method
rinpol	2742.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2771.00		NIST Webbook
rinpol	2801.00		NIST Webbook
rinpol	2742.00		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=R599610&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.