Benzo[a]pyrene, trans-7,8-diol, TMS

Inchi: InChI=1S/C26H28O2Si2/c1-29(2,3)27-22-14-12-17-11-13-21-20-10-8-7-9-18(20)15-19-1
InchiKey: WXSCTZVUFUMHAL-UHFFFAOYSA-N
Formula: C26H28O2Si2
SMILES: C[Si](C)(C)Oc1ccc2ccc3c4ccccc4cc4cc(O[Si](C)(C)C)c1c2c43
Mol. weight [g/mol]: 428.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.12		Crippen Method
logp	8.165		Crippen Method
rinpol	3137.00		NIST Webbook
rinpol	3144.00		NIST Webbook
rinpol	3151.00		NIST Webbook
rinpol	3137.00		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=R599625&Units=SI

Legend

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