cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3,4-dimethoxy, methylboronate

Inchi: InChI=1S/C18H19BO4/c1-18-13-8-6-5-7-11(13)15-12(17(18)22-19(2)23-18)9-10-14(20-3
InchiKey: TUIDUQPXILCRFN-MSOLQXFVSA-N
Formula: C18H19BO4
SMILES: COc1ccc2c(c1OC)-c1ccccc1C1(C)OB(C)OC21
Mol. weight [g/mol]: 310.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	3.805		Crippen Method
rinpol	2340.00		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=R109509&Units=SI

Legend

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