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

Inchi: InChI=1S/C17H17BO3/c1-17-15-7-5-4-6-12(15)14-10-11(19-3)8-9-13(14)16(17)20-18(2)2

InchiKey: XTJQHUZRJKMGGS-SJORKVTESA-N

Formula: C17H17BO3

SMILES: COc1ccc2c(c1)-c1ccccc1C1(C)OB(C)OC21

Mol. weight [g/mol]: 280.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	3.797		Crippen Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		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=R109554&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices