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

Inchi: InChI=1S/C20H23BO3/c1-4-5-12-21-23-19-16-11-10-14(22-3)13-17(16)15-8-6-7-9-18(15

InchiKey: WXDYLWHXPBUYEN-UXHICEINSA-N

Formula: C20H23BO3

SMILES: CCCCB1OC2c3ccc(OC)cc3-c3ccccc3C2(C)O1

Mol. weight [g/mol]: 322.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	4.967		Crippen Method
rinpol	2540.00		NIST Webbook
rinpol	2540.00		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=R109534&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices