cis-Phenanthrene, 9,10-dihydro-9,10-diol, methylboronate

Inchi: InChI=1S/C15H13BO2/c1-16-17-14-12-8-4-2-6-10(12)11-7-3-5-9-13(11)15(14)18-16/h2-9

InchiKey: YNTJDOULWYMRAF-GASCZTMLSA-N

Formula: C15H13BO2

SMILES: CB1OC2c3ccccc3-c3ccccc3C2O1

Mol. weight [g/mol]: 236.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	3.614		Crippen Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109445&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices