

# 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/ci9903071>  
Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

Latest version available from:

<https://www.chemeo.com/cid/19-147-8/cis-Phenanthrene-9-10-dihydro-9-methyl-9-10-diol-3-methoxy-butylboronate.p>

Generated by Cheméo on 2024-04-17 17:02:43.328193571 +0000 UTC m=+15662612.248770890.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.