

# trans-Phenanthrene, 9,10-dihydro-9,10-diol, butylboronate

**Inchi:** InChI=1S/C18H19BO2/c1-2-3-12-19-20-17-15-10-6-4-8-13(15)14-9-5-7-11-16(14)18(17)  
**InchiKey:** ZTXNKDBFIHNYIO-QZTJIDSGSA-N  
**Formula:** C18H19BO2  
**SMILES:** CCCCCB1OC2c3ccccc3-c3ccccc3C2O1  
**Mol. weight [g/mol]:** 278.15

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	4.784		Crippen Method
rinpol	2165.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109861&Units=SI>  
**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)

## Legend

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

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