

# trans-Anthracene, 1,2,3,4-tetrahydro-1,2-diol, butylboronate

Inchi:	InChI=1S/C18H21BO2/c1-2-3-10-19-20-17-9-8-15-11-13-6-4-5-7-14(13)12-16(15)18(17)
InchiKey:	YPPBZYZWJBTQAO-ROUUACIJSJSA-N
Formula:	C18H21BO2
SMILES:	CCCCB1OC2CCc3cc4ccccc4cc3C2O1
Mol. weight [g/mol]:	280.17

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	4.531		Crippen Method
rinpol	2290.00		NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R109712&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R109712&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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<https://www.chemeo.com/cid/66-060-2/trans-Anthracene-1-2-3-4-tetrahydro-1-2-diol-butylboronate.pdf>

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