

cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, 3,4-dimethoxy-butylboronate

InChI: InChI=1S/C21H25BO4/c1-5-6-13-22-25-20-15-11-12-17(23-3)19(24-4)18(15)14-9-7-8-10
InChIKey: VCCJDYVHZISQTRN-RTWAWAEBSA-N

Formula: C₂₁H₂₅BO₄

SMILES: CCCC(B1OC2c3ccc(OC)c(OC)c3-c3ccccc3C2(C)O1

Mol. weight [g/mol]: 352.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	4.976		Crippen Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109485&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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