

cis-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-HDICACEKSA-N
Formula: C18H19BO2
SMILES: CCCCC1OC2c3ccccc3-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	2180.00		NIST Webbook
rinpol	2180.00		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=R109425&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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<https://www.chemeo.com/cid/38-495-1/cis-Phenanthrene-9-10-dihydro-9-10-diol-butylboronate.pdf>

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