

cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, methylboronate

InChI: InChI=1S/C16H15BO2/c1-16-14-10-6-5-8-12(14)11-7-3-4-9-13(11)15(16)18-17(2)19-16/h
InChIKey: SPFLRXJREQHRMK-JKSUJKDBSA-N

Formula: C16H15BO2
SMILES: CB1OC2c3ccccc3-c3ccccc3C2(C)O1
Mol. weight [g/mol]: 250.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	3.788		Crippen Method
rinpol	1865.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109594&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/52-884-3/cis-Phenanthrene-9-10-dihydro-9-methyl-9-10-diol-methylboronate.pdf>

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