

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

Inchi:	InChI=1S/C15H13BO2/c1-16-17-14-12-8-4-2-6-10(12)11-7-3-5-9-13(11)15(14)18-16/h2-9
InchiKey:	YNTJDOULWYMRAF-GASCZTMLSA-N
Formula:	C15H13BO2
SMILES:	CB1OC2c3ccccc3-c3ccccc3C2O1
Mol. weight [g/mol]:	236.07

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	3.614		Crippen Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/47-602-1/cis-Phenanthrene-9-10-dihydro-9-10-diol-methylboronate.pdf>

Generated by Cheméo on 2024-05-02 02:34:20.628532508 +0000 UTC m=+16906509.549109824.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.