

cis-Anthracene, 1,2,3,4-tetrahydro-1,2-diol, methylboronate

Inchi: InChI=1S/C15H15BO2/c1-16-17-14-7-6-12-8-10-4-2-3-5-11(10)9-13(12)15(14)18-16/h2-5
InchiKey: NJQMHEASOUJRTC-CABCVRRESA-N
Formula: C15H15BO2
SMILES: CB1OC2CCc3cc4ccccc4cc3C2O1
Mol. weight [g/mol]: 238.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	3.360		Crippen Method
rinpol	1960.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109341&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/33-075-2/cis-Anthracene-1-2-3-4-tetrahydro-1-2-diol-methylboronate.pdf>

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