cis-Acenaphthen-1,2-diol, methylboronate

Inchi: InChI=1S/C13H11BO2/c1-14-15-12-9-6-2-4-8-5-3-7-10(11(8)9)13(12)16-14/h2-7,12-13H
InchiKey: CNGWVNBPEOSVSZ-BETUJISGSA-N
Formula: C13H11BO2
SMILES: CB1OC2c3cccc4cccc(c34)C2O1
Mol. weight [g/mol]: 210.04

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.01		Crippen Method
logp	3.100		Crippen Method
rinpol	1670.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109292&Units=SI

Legend

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