

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/ci9903071
Crippen Method:	https://www.cheméo.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

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