trans-Tetralin-2,3-diol, methylboronate

Inchi: InChI=1S/C11H13BO2/c1-12-13-10-6-8-4-2-3-5-9(8)7-11(10)14-12/h2-5,10-11H,6-7H2,1
InchiKey: PJNXJKWMVIXZEJ-QWRGUYRKSA-N
Formula: C11H13BO2
SMILES: CB1OC2Cc3ccccc3CC2O1
Mol. weight [g/mol]: 188.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.35		Crippen Method
logp	1.687		Crippen Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R109970&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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