cis-Indan-1,2-diol, methylboronate

Inchi: InChI=1S/C10H11BO2/c1-11-12-9-6-7-4-2-3-5-8(7)10(9)13-11/h2-5,9-10H,6H2,1H3/t9-,1
InchiKey: NNAFFLMVKWPWAR-ZJUUUORDSA-N
Formula: C10H11BO2
SMILES: CB1OC2Cc3ccccc3C2O1
Mol. weight [g/mol]: 174.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.28		Crippen Method
logp	1.817		Crippen Method
rinpol	1295.00		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=R109396&Units=SI

Legend

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