propyl-«delta»1-tetrahydrocannabinolic acid, methyl-boronate

Inchi: InChI=1S/C21H27BO4/c1-6-7-13-11-16-18(19-17(13)20(23)26-22(5)25-19)14-10-12(2)8-

InchiKey: SXKJWZVZFXKYKO-UHFFFAOYSA-N

Formula: C21H27BO4

SMILES: CCCc1cc2c(c3c1C(=O)OB(C)O3)C1C=C(C)CCC1C(C)(C)O2

Mol. weight [g/mol]: 354.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	4.917		Crippen Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R487597&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