«delta»1-tetrahydrocannabinolic acid, phenyl-boronate

Inchi: InChI=1S/C28H33BO4/c1-5-6-8-11-19-17-23-25(21-16-18(2)14-15-22(21)28(3,4)31-23)2

InchiKey: JYTYLNOWOXOGNE-UHFFFAOYSA-N

Formula: C28H33BO4

SMILES: CCCCCc1cc2c(c3c1C(=O)OB(c1ccccc1)O3)C1C=C(C)CCC1C(C)(C)O2

Mol. weight [g/mol]: 444.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.54		Crippen Method
logp	5.975		Crippen Method
rinpol	3404.00		NIST Webbook
rinpol	3404.00		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=R487502&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices