cannabidiolic acid, phenyl-boronate

Inchi: InChI=1S/C28H33BO4/c1-5-6-8-11-20-17-24(30)26(23-16-19(4)14-15-22(23)18(2)3)27-2
InchiKey: JJFDBRHKYHDRFR-PKTZIBPZSA-N
Formula: C28H33BO4
SMILES: C=C(C)C1CCC(C)=CC1c1c(O)cc(CCCCC)c2c1OB(c1ccccc1)OC2=O
Mol. weight [g/mol]: 444.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.23		Crippen Method
logp	6.085		Crippen Method
rinpol	3189.00		NIST Webbook
rinpol	3189.00		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=R487542&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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