propyl-«delta»1-tetrahydrocannabinolic acid, n-butyl-boronate

Inchi: InChI=1S/C24H33BO4/c1-6-8-12-25-28-22-20(23(26)29-25)16(9-7-2)14-19-21(22)17-13-

InchiKey: WILKJDZOTASJBN-UHFFFAOYSA-N

Formula: C24H33BO4

SMILES: CCCCB1OC(=O)c2c(CCC)cc3c(c2O1)C1C=C(C)CCC1C(C)(C)O3

Mol. weight [g/mol]: 396.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	6.088		Crippen Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		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=R487606&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices