

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)17-13-5
InchiKey: WILKJDZOTASJBN-UHFFFAOYSA-N
Formula: C24H33BO4
SMILES: CCCC(B1OC(=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/ci9903071>
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

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<https://www.chemeo.com/cid/57-329-4/propyl-delta-1-tetrahydrocannabinolic-acid-n-butyl-boronate.pdf>

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