

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	WILKJDZOTASJBN-UHFFFAOYSA-N
<b>Formula:</b>	C24H33BO4
<b>SMILES:</b>	CCCCB1OC(=O)c2c(CCC)cc3c(c2O1)C1C=C(C)CCC1C(C)(C)O3
<b>Mol. weight [g/mol]:</b>	396.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.78		Crippen Method
logp	6.088		Crippen Method
rinpol	2812.00		NIST Webbook
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## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R487606&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R487606&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>rinpol:</b>	Non-polar retention indices

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