

# propyl-«delta» 1-tetrahydrocannabinolic acid, methyl-boronate

<b>Inchi:</b>	InChI=1S/C21H27BO4/c1-6-7-13-11-16-18(19-17(13)20(23)26-22(5)25-19)14-10-12(2)8-
<b>InchiKey:</b>	SXKJWZVZFXKYKO-UHFFFAOYSA-N
<b>Formula:</b>	C21H27BO4
<b>SMILES:</b>	CCCc1cc2c(c3c1C(=O)OB(C)O3)C1C=C(C)CCC1C(C)(C)O2
<b>Mol. weight [g/mol]:</b>	354.25

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	4.917		Crippen Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R487597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R487597&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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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