

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

Inchi:	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-
InchiKey:	SXKJWZVZFXKYKO-UHFFFAOYSA-N
Formula:	C21H27BO4
SMILES:	CCCc1cc2c(c3c1C(=O)OB(C)O3)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]:	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

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=R487597&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/30-731-6/propyl-delta-1-tetrahydrocannabinolic-acid-methyl-boronate.pdf>

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