

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

Inchi:	InChI=1S/C26H37BO4/c1-6-8-10-11-18-16-21-23(19-15-17(3)12-13-20(19)26(4,5)29-21)
InchiKey:	MPEYXOZBJHRNIG-UHFFFAOYSA-N
Formula:	C26H37BO4
SMILES:	CCCCC1cc2c(c3c1C(=O)OB(CCCC)O3)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]:	424.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	6.868		Crippen Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R487493&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/88-223-7/delta-1-tetrahydrocannabinolic-acid-n-butyl-boronate.pdf>

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