

«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: CCCCCc1cc2c(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
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487493&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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