

«delta»1-tetrahydrocannabinolic acid, methyl-boronate

Inchi: InChI=1S/C23H31BO4/c1-6-7-8-9-15-13-18-20(21-19(15)22(25)28-24(5)27-21)16-12-14
InchiKey: CNEUKTJXBAJPGS-UHFFFAOYSA-N
Formula: C23H31BO4
SMILES: CCCCCc1cc2c(c3c1C(=O)OB(C)O3)C1C=C(C)CCC1C(C)(C)O2
Mol. weight [g/mol]: 382.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	5.697		Crippen Method
rinpol	2725.00		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=R487488&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/97-285-9/delta-1-tetrahydrocannabinolic-acid-methyl-boronate.pdf>

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