

Brassinolide, methaneboronate

Inchi: InChI=1S/C29H48B2O6/c1-15(2)16(3)24-25(37-31(8)36-24)17(4)18-9-10-19-26-20(11-12)28-27-23-22-21-20
InchiKey: WNAFVLJYKMGAN-GSIHARNGSA-N
Formula: C₂₉H₄₈B₂O₆
SMILES: CB1OC2CC3C(=O)OC4C(CCC5(C)C(C(C)C6OB(C)OC6C(C)C(C)C)CCC45)C3(C)CC2O
Mol. weight [g/mol]: 514.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	5.503		Crippen Method
rinpol	3723.00		NIST Webbook
rinpol	3724.00		NIST Webbook
rinpol	3723.00		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=R497173&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/48-694-9/Brassinolide-methaneboronate.pdf>

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