

trans-Tetralin-2,3-diol, butylboronate

Inchi: InChI=1S/C14H19BO2/c1-2-3-8-15-16-13-9-11-6-4-5-7-12(11)10-14(13)17-15/h4-7,13-14
InchiKey: BJHRXOCAFPZFSY-KBPBESRZSA-N
Formula: C14H19BO2
SMILES: CCCC(B1OC2Cc3ccccc3CC2O1)
Mol. weight [g/mol]: 230.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	2.857		Crippen Method
rinpol	1730.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R109950&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/29-086-5/trans-Tetralin-2-3-diol-butylboronate.pdf>

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