

trans-Tetralin-2,3-diol, methylboronate

Inchi:	InChI=1S/C11H13BO2/c1-12-13-10-6-8-4-2-3-5-9(8)7-11(10)14-12/h2-5,10-11H,6-7H2,1
InchiKey:	PJNXJKWVMVIXZEJ-QWRGUYRKSA-N
Formula:	C11H13BO2
SMILES:	CB1OC2Cc3ccccc3CC2O1
Mol. weight [g/mol]:	188.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.35		Crippen Method
logp	1.687		Crippen Method
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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<https://www.cheméo.com/cid/23-929-5/trans-Tetralin-2-3-diol-methylboronate.pdf>

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