

trans-Tetralin-1,2-diol, methylboronate

Inchi:	InChI=1S/C11H13BO2/c1-12-13-10-7-6-8-4-2-3-5-9(8)11(10)14-12/h2-5,10-11H,6-7H2,1
InchiKey:	ZMVIKJBMRGOUEP-GHMZBOCLSA-N
Formula:	C11H13BO2
SMILES:	CB1OC2CCc3ccccc3C2O1
Mol. weight [g/mol]:	188.03

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	2.207		Crippen Method
rinpol	1445.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/64-438-5/trans-Tetralin-1-2-diol-methylboronate.pdf>

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