

Ethanediol, hexylboronate

Inchi:	InChI=1S/C8H17BS2/c1-2-3-4-5-6-9-10-7-8-11-9/h2-8H2,1H3
InchiKey:	ORLRWYSMQRMPIM-UHFFFAOYSA-N
Formula:	C8H17BS2
SMILES:	CCCCCB1SCCS1
Mol. weight [g/mol]:	188.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	3.535		Crippen Method
rinpol	1123.00		NIST Webbook
rinpol	1117.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62118&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/51-410-9/Ethanediol-hexylboronate.pdf>

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