

Ethanediol, pentylboronate

Inchi: InChI=1S/C7H15BS2/c1-2-3-4-5-8-9-6-7-10-8/h2-7H2,1H3
InchiKey: DBSLIRDLDKWHZRJ-UHFFFAOYSA-N
Formula: C7H15BS2
SMILES: CCCCCB1SCCS1
Mol. weight [g/mol]: 174.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.08		Crippen Method
logp	3.145		Crippen Method
rinpol	1023.00		NIST Webbook
rinpol	1020.00		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=R62122&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/14-949-3/Ethanediol-pentylboronate.pdf>

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