

Ethanediol, butylboronate

Inchi: InChI=1S/C6H13BS2/c1-2-3-4-7-8-5-6-9-7/h2-6H2,1H3
InchiKey: FPEVZPSEKLPDCO-UHFFFAOYSA-N
Formula: C6H13BS2
SMILES: CCCCC1SCCS1
Mol. weight [g/mol]: 160.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.66		Crippen Method
logp	2.755		Crippen Method
rinpol	914.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62097&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

Latest version available from:

<https://www.cheméo.com/cid/24-828-6/Ethanediol-butylboronate.pdf>

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