4-iodobutaneboronate, mephenesin

Inchi: InChI=1S/C16H16BIO3/c1-12-4-2-3-5-16(12)19-10-15-11-20-17(21-15)13-6-8-14(18)9-7-

InchiKey: WGFZPWGCRQNIMN-UHFFFAOYSA-N

Formula: C16H16BIO3

SMILES: Cc1ccccc1OCC1COB(c2ccc(I)cc2)O1

Mol. weight [g/mol]: 394.01

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.49		Crippen Method
logp	2.789		Crippen Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R146766&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices