

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:	Cc1cccc1OCC1COB(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

Latest version available from:

<https://www.chemeo.com/cid/121-142-9/4-iodobutaneboronate-mephenesin.pdf>

Generated by Cheméo on 2024-11-09 10:03:47.455342427 +0000 UTC m=+5727490.092311676.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.