

2,4-Dichlorobenzeneboronate, mephenesin

Inchi: InChI=1S/C16H15BCl2O3/c1-11-4-2-3-5-16(11)20-9-13-10-21-17(22-13)14-7-6-12(18)8-
InchiKey: VQSFUHCENLSPKY-UHFFFAOYSA-N
Formula: C16H15BCl2O3
SMILES: Cc1ccccc1OCC1COB(c2ccc(Cl)cc2Cl)O1
Mol. weight [g/mol]: 337.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.72		Crippen Method
logp	3.491		Crippen Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R146706&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/122-515-4/2-4-Dichlorobenzeneboronate-mephenesin.pdf>

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