

Benzeneboronic acid, m-nitro-

Other names:	Boronic acid, B-(3-nitrophenyl)- 3-NITROPHENYLBORONIC ACID
Inchi:	InChI=1S/C6H6BNO4/c9-7(10)5-2-1-3-6(4-5)8(11)12/h1-4,9-10H
InchiKey:	ZNRGSYUVFVNSAW-UHFFFAOYSA-N
Formula:	C6H6BNO4
SMILES:	O=[N+](O)c1cccc(B(O)O)c1
Mol. weight [g/mol]:	166.93
CAS:	13331-27-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	-0.725		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13331276&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

Latest version available from:

<https://www.chemeo.com/cid/73-073-0/Benzeneboronic-acid-m-nitro.pdf>

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