

benzeneboronic acid

Other names:	phenylboric acid phenylboronic acid
Inchi:	InChI=1S/C6H7BO2/c8-7(9)6-4-2-1-3-5-6/h1-5,8-9H
InchiKey:	HXITXNWTGFUOAU-UHFFFAOYSA-N
Formula:	C6H7BO2
SMILES:	OB(O)c1ccccc1
Mol. weight [g/mol]:	121.93

Physical Properties

Property code	Value	Unit	Source
ie	9.55	eV	Cheméo Relay (1.0)
logp	-0.634		Crippen Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Solubilities of 4-Phenyltoluene, Phenylboric Acid, Biphenyl, and Carbon Dioxide from Measurements of the Relative Permittivity:

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/105-459-6/benzeneboronic-acid.pdf>

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