

p-Methylbenzeneboronic acid

Other names:	Boronic acid, (4-methylphenyl)- Boronic acid, B-(4-methylphenyl)- Boronic acid, p-tolyl- p-Tolueneboronic acid p-Tolylboronic acid
Inchi:	InChI=1S/C7H9BO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5,9-10H,1H3
InchiKey:	BIWQNIMLAISTBV-UHFFFAOYSA-N
Formula:	C7H9BO2
SMILES:	Cc1ccc(B(O)O)cc1
Mol. weight [g/mol]:	135.96
CAS:	5720-05-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	-0.325		Crippen Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5720058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubilities of p-Tolylboronic Acid, Bromobenzene and 4-Phenyltoluene in Carbon Dioxide at Elevated Pressures:	https://www.doi.org/10.1021/je034051y

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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<https://www.chemeo.com/cid/21-989-1/p-Methylbenzeneboronic-acid.pdf>

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