

Catecholborane

Other names:	1,3,2-Benzodioxaborole Pyrocatecholborane Benzcatechinborane Catecholatorborane
Inchi:	InChI=1S/C6H5BO2/c1-2-4-6-5(3-1)8-7-9-6/h1-4,7H
InchiKey:	CENMEJUYOOMFFZ-UHFFFAOYSA-N
Formula:	C6H5BO2
SMILES:	B1Oc2ccccc2O1
Mol. weight [g/mol]:	119.91
CAS:	274-07-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.78		Crippen Method
logp	0.724		Crippen Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C274077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/77-838-7/Catecholborane.pdf>

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