

1-Butaneboronic acid

Other names:	Butylboronic acid Butylboric acid n-Butaneboronic acid Boronic acid, butyl- 1-butyldihydroxyborane Dihydroxy-n-butylborane
Inchi:	InChI=1S/C4H11BO2/c1-2-3-4-5(6)7/h6-7H,2-4H2,1H3
InchiKey:	QPKFVRWIIEVCW-UHFFFAOYSA-N
Formula:	C4H11BO2
SMILES:	CCCCB(O)O
Mol. weight [g/mol]:	101.94
CAS:	4426-47-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.31		Crippen Method
logp	0.259		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	69.90 ± 0.80	kJ/mol	321.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4426475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hsubt: Enthalpy of sublimation at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

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