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:	QPKFVRWIISEVCW-UHFFFAOYSA-N
Formula:	C4H11BO2
SMILES:	CCCCB(O)O
Mol. weight [g/mol]:	101.94

Physical Properties

Property code	Value	Unit	Source
af	0.7643		Cheméo Relay (1.0)
gf	-371.13	kJ/mol	Cheméo Relay (1.0, beta)
hf	-626.00	kJ/mol	Cheméo Relay (1.0)
hvap	59.13	kJ/mol	Cheméo Relay (1.0)
ie	10.36	eV	Cheméo Relay (1.0)
log10ws	0.06		Cheméo Relay (1.0)
logp	0.259		Crippen Method
pc	5502.62	kPa	Cheméo Relay (1.0, beta)
tb	468.44	K	Cheméo Relay (1.0)
tc	650.04	K	Cheméo Relay (1.0)
tf	334.87	K	Cheméo Relay (1.0)
vc	0.341	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4426475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume