

Borane(1)

Inchi: InChI=1S/BH/h1H
InchiKey: UWBOAQKPEXKXSU-UHFFFAOYSA-N
Formula: BH
SMILES: [BH]
Mol. weight [g/mol]: 11.82
CAS: 13766-26-2

Physical Properties

Property code	Value	Unit	Source
ea	0.30 ± 0.25	eV	NIST Webbook
ie	9.77	eV	NIST Webbook
ie	9.80 ± 0.50	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
ie	9.77 ± 0.05	eV	NIST Webbook
log10ws	2.83		Crippen Method
logp	-0.649		Crippen Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13766262&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ea: Electron affinity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

Latest version available from:

<https://www.chemeo.com/cid/15-354-2/Borane-1.pdf>

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