

9b-Boraphenalene, dodecahydro-

Other names:	Zentrobor,l perhydro-9b-boraphenalene Dodecahydro-9-boraphenalene
Inchi:	InChI=1S/C12H21B/c1-4-10-6-2-8-12-9-3-7-11(5-1)13(10)12/h10-12H,1-9H2
InchiKey:	SKOKKTJRHJQZHK-UHFFFAOYSA-N
Formula:	C12H21B
SMILES:	C1CC2CCCC3CCCC(C1)B23
Mol. weight [g/mol]:	176.11
CAS:	16664-33-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	4.144		Crippen Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	53.10	kJ/mol	354.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16664338&Units=SI

Legend

hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

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