

Selenium hexamer

Other names:	Cyclic hexaatomic selenium
Inchi:	InChI=1S/Se6/c1-2-4-6-5-3-1
InchiKey:	FBNWFNKLBDQILL-UHFFFAOYSA-N
Formula:	Se6
SMILES:	[Se]1[Se][Se][Se][Se][Se]1
Mol. weight [g/mol]:	473.76
CAS:	12597-30-7

Physical Properties

Property code	Value	Unit	Source
ie	8.23 ± 0.05	eV	NIST Webbook
ie	9.08 ± 0.05	eV	NIST Webbook
ie	8.90 ± 0.20	eV	NIST Webbook
log10ws	14.01		Crippen Method
logp	-2.285		Crippen Method

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=C12597307&Units=SI

Legend

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/37-235-0/Selenium-hexamer.pdf>

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