

Selenophene, 2-(methylthio)-

Other names:	2-(Methylthio)selenophene
Inchi:	InChI=1S/C5H6SSe/c1-6-5-3-2-4-7-5/h2-4H,1H3
InchiKey:	KDJCFNABGJTVEI-UHFFFAOYSA-N
Formula:	C5H6SSe
SMILES:	CSc1ccc[se]1
Mol. weight [g/mol]:	177.13
CAS:	31053-54-0

Physical Properties

Property code	Value	Unit	Source
ie	8.75	eV	NIST Webbook
log10ws	0.66		Crippen Method
logp	1.466		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=C31053540&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/91-555-5/Selenophene-2-methylthio.pdf>

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