

Methyl isoselenocyanate

Inchi:	InChI=1S/C2H3NSe/c1-3-2-4/h1H3
InchiKey:	PBYQRKLVFZCKNK-UHFFFAOYSA-N
Formula:	C2H3NSe
SMILES:	CN=C=[SeH]
Mol. weight [g/mol]:	120.01
CAS:	4426-70-4

Physical Properties

Property code	Value	Unit	Source
ie	8.90	eV	NIST Webbook
log10ws	2.82		Crippen Method
logp	-0.578		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=C4426704&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/81-205-4/Methyl-isoselenocyanate.pdf>

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