

# Trimethylsilyl isothiocyanate

<b>Other names:</b>	Silane, isothiocyanatotrimethyl-
<b>Inchi:</b>	InChI=1S/C4H9NSSi/c1-7(2,3)5-4-6/h1-3H3
<b>InchiKey:</b>	XLTUPERVRFLGLJ-UHFFFAOYSA-N
<b>Formula:</b>	C4H9NSSi
<b>SMILES:</b>	C[Si](C)(C)N=C=S
<b>Mol. weight [g/mol]:</b>	131.27
<b>CAS:</b>	2290-65-5

## Physical Properties

Property code	Value	Unit	Source
ie	9.26	eV	NIST Webbook
ie	9.30 ± 0.10	eV	NIST Webbook
log10ws	0.52		Crippen Method
logp	1.924		Crippen Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2290655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2290655&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

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<https://www.chemeo.com/cid/57-259-2/Trimethylsilyl-isothiocyanate.pdf>

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