

2-Thiocytosine, TMS

Other names:	Pyrimidine, 4-amino-2-mercapto, TMS
Inchi:	InChI=1S/C10H21N3SSi2/c1-15(2,3)13-9-7-8-11-10(12-9)14-16(4,5)6/h7-8H,1-6H3,(H,1
InchiKey:	IQKSHKCJKQQMLH-UHFFFAOYSA-N
Formula:	C10H21N3SSi2
SMILES:	C[Si](C)(C)Nc1ccnc(S[Si](C)(C)C)n1
Mol. weight [g/mol]:	271.53

Physical Properties

Property code	Value	Unit	Source
log10ws	0.47		Crippen Method
logp	3.650		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R93618&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

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