

2,4-Dithiothymine, TMS

Inchi:	InChI=1S/C11H22N2S2Si2/c1-9-8-12-11(15-17(5,6)7)13-10(9)14-16(2,3)4/h8H,1-7H3
InchiKey:	UQLKKIJAGOJFDD-UHFFFAOYSA-N
Formula:	C11H22N2S2Si2
SMILES:	Cc1cnc(S[Si](C)(C)C)nc1S[Si](C)(C)C
Mol. weight [g/mol]:	302.61

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	4.639		Crippen Method
rinpol	1768.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R93551&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/54-676-2/2-4-Dithiothymine-TMS.pdf>

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