

# Homocystine, TMS # 1

**Inchi:** InChI=1S/C20H48N2O4S2Si4/c1-29(2,3)21-17(19(23)25-31(7,8)9)13-15-27-28-16-14-18  
**InchiKey:** VVODJOVRLCDBOE-UHFFFAOYSA-N  
**Formula:** C20H48N2O4S2Si4  
**SMILES:** C[Si](C)(C)NC(CCSSCCC(N[Si](C)(C)C)C(=O)O[Si](C)(C)C(=O)O[Si](C)(C)C  
**Mol. weight [g/mol]:** 557.08

## Physical Properties

Property code	Value	Unit	Source
log10ws	2.52		Crippen Method
logp	5.490		Crippen Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401033&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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/112-889-1/Homocystine-TMS-1.pdf>

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