

# Morpholinecarbodithioic acid, 3,3'-dithiodipropyl ester

**Inchi:** InChI=1S/C16H28N2O2S6/c21-15(17-3-7-19-8-4-17)23-11-1-13-25-26-14-2-12-24-16(22-16)  
**InchiKey:** MSUQUUHVVRJDFE-UHFFFAOYSA-N  
**Formula:** C16H28N2O2S6  
**SMILES:** S=C(SCCCSSCCCSC(=S)N1CCOCC1)N1CCOCC1  
**Mol. weight [g/mol]:** 472.80  
**CAS:** 64226-39-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	3.849		Crippen Method
mcvol	335.780	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64226397&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  
**mcvol:** McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/116-584-5/Morpholinecarbodithioic-acid-3-3-dithiodipropyl-ester.pdf>

Generated by Cheméo on 2024-04-28 08:30:02.797959619 +0000 UTC m=+16582251.718536934.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.