

# Phenylthioacetic acid, morpholide

**Inchi:** InChI=1S/C12H15NO2S/c14-12(13-6-8-15-9-7-13)10-16-11-4-2-1-3-5-11/h1-5H,6-10H2  
**InchiKey:** NAMFKTBQSCMITK-UHFFFAOYSA-N  
**Formula:** C12H15NO2S  
**SMILES:** O=C(CSc1ccccc1)N1CCOCC1  
**Mol. weight [g/mol]:** 237.32

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.638		Crippen Method
mcvol	179.090	ml/mol	McGowan Method
rinpol	2038.00		NIST Webbook
rinpol	2038.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307203&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices

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