

# Simetryn sylfone

**Inchi:** InChI=1S/C8H15N5O2S/c1-4-9-6-11-7(10-5-2)13-8(12-6)16(3,14)15/h4-5H2,1-3H3,(H2,S)  
**InchiKey:** FZIFQDDMRNBIGA-UHFFFAOYSA-N  
**Formula:** C8H15N5O2S  
**SMILES:** CCNc1nc(NCC)nc(S(C)(=O)=O)n1  
**Mol. weight [g/mol]:** 245.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.32		Crippen Method
logp	0.139		Crippen Method
mcvol	177.810	ml/mol	McGowan Method
rinpola	2216.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R543776&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

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

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