

# Sertraline

**Other names:**

(1S,4S)-4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydro-N-methyl-1-naphthalenamine  
(1S,4S)-4-(3,4-Dichlorophenyl)-1,2,3,4-tetrahydro-N-methyl-1-naphthylamine  
(1S-cis)-1,2,3,4-Tetrahydro-4-(3,4-dichlorophenyl)-N-methyl-1-naphthalenamine  
CP 51974  
79559-97-0 (hydrochloride)

**Inchi:** InChI=1S/C17H17Cl2N/c1-20-17-9-7-12(13-4-2-3-5-14(13)17)11-6-8-15(18)16(19)10-11/**InchiKey:** VGKDLMBJGBXTGI-UHFFFAOYSA-N**Formula:** C17H17Cl2N**SMILES:** CNC1CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21**Mol. weight [g/mol]:** 306.23**CAS:** 79617-96-2

## Physical Properties

Property code	Value	Unit	Source
gf	394.66	kJ/mol	Joback Method
hf	112.73	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	74.96	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.180		Crippen Method
mcvol	226.470	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
tb	788.03	K	Joback Method
tc	1041.02	K	Joback Method
tf	494.43	K	Joback Method
vc	0.853	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.18	J/molxK	788.03	Joback Method
cpg	639.33	J/molxK	830.20	Joback Method
cpg	654.14	J/molxK	872.36	Joback Method
cpg	667.70	J/molxK	914.53	Joback Method

cpg	680.12	J/mol×K	956.69	Joback Method
cpg	691.51	J/mol×K	998.86	Joback Method
cpg	701.99	J/mol×K	1041.02	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C79617962&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C79617962&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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