

# Sertraline, ketone

<b>Inchi:</b>	InChI=1S/C16H12Cl2O/c17-14-7-5-10(9-15(14)18)11-6-8-16(19)13-4-2-1-3-12(11)13/h1-
<b>InchiKey:</b>	JGMBHJNMQVKDMW-LLVKDONJSA-N
<b>Formula:</b>	C16H12Cl2O
<b>SMILES:</b>	O=C1CCC(c2ccc(Cl)c(Cl)c2)c2ccccc21
<b>Mol. weight [g/mol]:</b>	291.17

## Physical Properties

Property code	Value	Unit	Source
gf	181.97	kJ/mol	Joback Method
hf	-37.46	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.102		Crippen Method
mcvol	203.970	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rmpol	2480.00		NIST Webbook
tb	787.47	K	Joback Method
tc	1060.11	K	Joback Method
tf	502.96	K	Joback Method
vc	0.769	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.55	J/mol×K	787.47	Joback Method
cpg	552.57	J/mol×K	832.91	Joback Method
cpg	566.13	J/mol×K	878.35	Joback Method
cpg	578.30	J/mol×K	923.79	Joback Method
cpg	589.16	J/mol×K	969.23	Joback Method
cpg	598.77	J/mol×K	1014.67	Joback Method
cpg	607.22	J/mol×K	1060.11	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R196073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R196073&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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