

# L-Serine, N,O-bis(2-chlorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C18H15Cl2NO5/c1-25-18(24)15(21-16(22)11-6-2-4-8-13(11)19)10-26-17(23)1
<b>InchiKey:</b>	XKVADCVCQJNALI-UHFFFAOYSA-N
<b>Formula:</b>	C18H15Cl2NO5
<b>SMILES:</b>	<chem>COC(=O)C(COC(=O)c1ccccc1Cl)NC(=O)c1ccccc1Cl</chem>
<b>Mol. weight [g/mol]:</b>	396.22

## Physical Properties

Property code	Value	Unit	Source
gf	-227.43	kJ/mol	Joback Method
hf	-550.20	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	101.41	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.122		Crippen Method
mcvol	267.870	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
tb	1005.60	K	Joback Method
tc	1250.41	K	Joback Method
tf	662.25	K	Joback Method
vc	1.008	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.04	J/molxK	1005.60	Joback Method
cpg	771.84	J/molxK	1046.40	Joback Method
cpg	778.31	J/molxK	1087.20	Joback Method
cpg	783.49	J/molxK	1128.00	Joback Method
cpg	787.43	J/molxK	1168.81	Joback Method
cpg	790.15	J/molxK	1209.61	Joback Method
cpg	791.71	J/molxK	1250.41	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=U299592&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299592&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>hvap:</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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