

# L-Methionine, N-(2-chlorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C13H16ClNO3S/c1-18-13(17)11(7-8-19-2)15-12(16)9-5-3-4-6-10(9)14/h3-6,11
InchiKey:	VTGMWNUUHTXXLY-UHFFFAOYSA-N
Formula:	C13H16ClNO3S
SMILES:	COC(=O)C(CCSC)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	301.79

## Physical Properties

Property code	Value	Unit	Source
gf	-93.34	kJ/mol	Joback Method
hf	-369.65	kJ/mol	Joback Method
hfus	37.37	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.365		Crippen Method
mvol	217.850	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	814.60	K	Joback Method
tc	1045.47	K	Joback Method
tf	499.28	K	Joback Method
vc	0.818	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.83	J/mol×K	814.60	Joback Method
cpg	601.74	J/mol×K	853.08	Joback Method
cpg	612.54	J/mol×K	891.56	Joback Method
cpg	622.27	J/mol×K	930.04	Joback Method
cpg	630.95	J/mol×K	968.51	Joback Method
cpg	638.58	J/mol×K	1006.99	Joback Method
cpg	645.21	J/mol×K	1045.47	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U299590&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299590&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>rinp:</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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