

# Sarcosine, N-(4-chlorobenzoyl)-, propyl ester

<b>Inchi:</b>	InChI=1S/C13H16ClNO3/c1-3-8-18-12(16)9-15(2)13(17)10-4-6-11(14)7-5-10/h4-7H,3,8-9
<b>InchiKey:</b>	IHSZLSTUMANN CN-UHFFFAOYSA-N
<b>Formula:</b>	C13H16ClNO3
<b>SMILES:</b>	CCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	269.72

## Physical Properties

Property code	Value	Unit	Source
gf	-102.63	kJ/mol	Joback Method
hf	-392.18	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.365		Crippen Method
mvol	201.500	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	708.53	K	Joback Method
tc	919.99	K	Joback Method
tf	459.69	K	Joback Method
vc	0.752	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.21	J/mol×K	708.53	Joback Method
cpg	539.60	J/mol×K	743.77	Joback Method
cpg	552.07	J/mol×K	779.02	Joback Method
cpg	563.66	J/mol×K	814.26	Joback Method
cpg	574.38	J/mol×K	849.50	Joback Method
cpg	584.29	J/mol×K	884.75	Joback Method
cpg	593.39	J/mol×K	919.99	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=U321347&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321347&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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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