

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

<b>Inchi:</b>	InChI=1S/C18H26ClNO3/c1-3-4-5-6-7-8-13-23-17(21)14-20(2)18(22)15-9-11-16(19)12-1
<b>InchiKey:</b>	DRFOMTJWBVHUCF-UHFFFAOYSA-N
<b>Formula:</b>	C18H26ClNO3
<b>SMILES:</b>	CCCCCCCCOC(=O)CN(C)C(=O)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	339.86

## Physical Properties

Property code	Value	Unit	Source
gf	-60.53	kJ/mol	Joback Method
hf	-495.38	kJ/mol	Joback Method
hfus	47.63	kJ/mol	Joback Method
hvap	80.93	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.316		Crippen Method
mvol	271.950	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	822.93	K	Joback Method
tc	1026.04	K	Joback Method
tf	516.04	K	Joback Method
vc	1.032	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.68	J/mol×K	822.93	Joback Method
cpg	816.68	J/mol×K	856.78	Joback Method
cpg	830.65	J/mol×K	890.63	Joback Method
cpg	843.63	J/mol×K	924.49	Joback Method
cpg	855.66	J/mol×K	958.34	Joback Method
cpg	866.79	J/mol×K	992.19	Joback Method
cpg	877.06	J/mol×K	1026.04	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=U321354&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321354&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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