

# Sarcosine, N-(4-nitrobenzoyl)-, nonyl ester

<b>Inchi:</b>	InChI=1S/C19H28N2O5/c1-3-4-5-6-7-8-9-14-26-18(22)15-20(2)19(23)16-10-12-17(13-11
<b>InchiKey:</b>	WHGAPBZZOFDLPC-UHFFFAOYSA-N
<b>Formula:</b>	C19H28N2O5
<b>SMILES:</b>	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	364.44

## Physical Properties

Property code	Value	Unit	Source
gf	-4.63	kJ/mol	Joback Method
hf	-511.04	kJ/mol	Joback Method
hfus	57.39	kJ/mol	Joback Method
hvap	95.36	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.961		Crippen Method
mcvol	291.220	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinqol	3002.00		NIST Webbook
tb	960.22	K	Joback Method
tc	1182.55	K	Joback Method
tf	641.00	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.56	J/molxK	960.22	Joback Method
cpg	957.86	J/molxK	997.28	Joback Method
cpg	970.01	J/molxK	1034.33	Joback Method
cpg	981.07	J/molxK	1071.39	Joback Method
cpg	991.10	J/molxK	1108.44	Joback Method
cpg	1000.17	J/molxK	1145.50	Joback Method
cpg	1008.33	J/molxK	1182.55	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=U321288&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321288&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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