

# Sarcosine, N-(3-methoxybenzoyl)-, nonyl ester

<b>Inchi:</b>	InChI=1S/C20H31NO4/c1-4-5-6-7-8-9-10-14-25-19(22)16-21(2)20(23)17-12-11-13-18(15)
<b>InchiKey:</b>	DFHNPWMYNUAEVFN-UHFFFAOYSA-N
<b>Formula:</b>	C20H31NO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CN(C)C(=O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	349.46

## Physical Properties

Property code	Value	Unit	Source
gf	-136.76	kJ/mol	Joback Method
hf	-653.14	kJ/mol	Joback Method
hfus	49.80	kJ/mol	Joback Method
hvap	83.41	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.061		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2731.00		NIST Webbook
rinpol	2731.00		NIST Webbook
tb	853.68	K	Joback Method
tc	1053.86	K	Joback Method
tf	530.89	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.18	J/mol×K	853.68	Joback Method
cpg	936.33	J/mol×K	887.04	Joback Method
cpg	951.33	J/mol×K	920.41	Joback Method
cpg	965.21	J/mol×K	953.77	Joback Method
cpg	978.00	J/mol×K	987.13	Joback Method
cpg	989.73	J/mol×K	1020.50	Joback Method
cpg	1000.44	J/mol×K	1053.86	Joback Method

# Sources

<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=U321498&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321498&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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

Latest version available from:

<https://www.cheméo.com/cid/69-107-7/Sarcosine-N-3-methoxybenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-19 15:13:11.866202929 +0000 UTC m=+15828840.786780251.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.