

# Sarcosine, N-(2-methylbenzoyl)-, hexadecyl ester

Inchi:	InChI=1S/C27H45NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-31-26(29)23-28(3)27
InchiKey:	OEGIUOJXEVOGIL-UHFFFAOYSA-N
Formula:	C27H45NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1C
Mol. weight [g/mol]:	431.65

## Physical Properties

Property code	Value	Unit	Source
gf	27.18	kJ/mol	Joback Method
hf	-665.40	kJ/mol	Joback Method
hfus	66.75	kJ/mol	Joback Method
hvap	96.58	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	7.092		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	871.71	kPa	Joback Method
tb	991.42	K	Joback Method
tc	1215.43	K	Joback Method
tf	587.55	K	Joback Method
vc	1.488	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1320.83	J/molxK	991.42	Joback Method
cpg	1339.62	J/molxK	1028.75	Joback Method
cpg	1356.95	J/molxK	1066.09	Joback Method
cpg	1372.90	J/molxK	1103.42	Joback Method
cpg	1387.57	J/molxK	1140.76	Joback Method
cpg	1401.03	J/molxK	1178.09	Joback Method
cpg	1413.37	J/molxK	1215.43	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=U321176&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321176&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>
<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>hvap:</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>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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