

# Sarcosine, N-(2-methoxybenzoyl)-, pentyl ester

Inchi:	InChI=1S/C16H23NO4/c1-4-5-8-11-21-15(18)12-17(2)16(19)13-9-6-7-10-14(13)20-3/h6-
InchiKey:	UAGSTRSFJYLKQD-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCCCCOC(=O)CN(C)C(=O)c1ccccc1OC
Mol. weight [g/mol]:	293.36

## Physical Properties

Property code	Value	Unit	Source
gf	-170.44	kJ/mol	Joback Method
hf	-570.58	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	74.50	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.501		Crippen Method
mvol	237.400	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	762.16	K	Joback Method
tc	962.44	K	Joback Method
tf	485.81	K	Joback Method
vc	0.889	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.07	J/molxK	762.16	Joback Method
cpg	704.28	J/molxK	795.54	Joback Method
cpg	718.48	J/molxK	828.92	Joback Method
cpg	731.71	J/molxK	862.30	Joback Method
cpg	743.96	J/molxK	895.68	Joback Method
cpg	755.28	J/molxK	929.06	Joback Method
cpg	765.67	J/molxK	962.44	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321145&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321145&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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