

# Sarcosine, n-hexanoyl-, octyl ester

<b>Inchi:</b>	InChI=1S/C17H33NO3/c1-4-6-8-9-10-12-14-21-17(20)15-18(3)16(19)13-11-7-5-2/h4-15H
<b>InchiKey:</b>	ZXWZUZMQURKFNG-UHFFFAOYSA-N
<b>Formula:</b>	C17H33NO3
<b>SMILES:</b>	CCCCCCCCOC(=O)CN(C)C(=O)CCCCC
<b>Mol. weight [g/mol]:</b>	299.45

## Physical Properties

Property code	Value	Unit	Source
gf	-159.80	kJ/mol	Joback Method
hf	-684.06	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.929		Crippen Method
mcvol	269.380	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpola	2197.00		NIST Webbook
tb	730.96	K	Joback Method
tc	906.84	K	Joback Method
tf	435.91	K	Joback Method
vc	1.036	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.22	J/mol×K	730.96	Joback Method
cpg	819.60	J/mol×K	760.27	Joback Method
cpg	836.10	J/mol×K	789.59	Joback Method
cpg	851.75	J/mol×K	818.90	Joback Method
cpg	866.57	J/mol×K	848.21	Joback Method
cpg	880.59	J/mol×K	877.53	Joback Method
cpg	893.82	J/mol×K	906.84	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=U321126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321126&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.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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