

# Sarcosine, N-(3-cyclopentylpropionyl)-, hexyl ester

Inchi:	InChI=1S/C17H31NO3/c1-3-4-5-8-13-21-17(20)14-18(2)16(19)12-11-15-9-6-7-10-15/h15
InchiKey:	ZSZTYULFXLYSOU-UHFFFAOYSA-N
Formula:	C17H31NO3
SMILES:	CCCCCOC(=O)CN(C)C(=O)CCC1CCCC1
Mol. weight [g/mol]:	297.43

## Physical Properties

Property code	Value	Unit	Source
gf	-123.25	kJ/mol	Joback Method
hf	-623.58	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	71.64	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.539		Crippen Method
mvol	258.520	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	746.24	K	Joback Method
tc	936.47	K	Joback Method
tf	446.81	K	Joback Method
vc	0.977	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.64	J/mol×K	746.24	Joback Method
cpg	813.10	J/mol×K	777.94	Joback Method
cpg	830.49	J/mol×K	809.65	Joback Method
cpg	846.83	J/mol×K	841.35	Joback Method
cpg	862.16	J/mol×K	873.06	Joback Method
cpg	876.53	J/mol×K	904.76	Joback Method
cpg	889.96	J/mol×K	936.47	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=U321835&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321835&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>

# 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>rinpola:</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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