

# Sarcosine, N-valeryl-, pentadecyl ester

<b>Inchi:</b>	InChI=1S/C23H45NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-20-27-23(26)21-24(3)22
<b>InchiKey:</b>	LEKUGSRCJMNXQC-UHFFFAOYSA-N
<b>Formula:</b>	C23H45NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)CCCC
<b>Mol. weight [g/mol]:</b>	383.61

## Physical Properties

Property code	Value	Unit	Source
gf	-109.28	kJ/mol	Joback Method
hf	-807.90	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.269		Crippen Method
mcvol	353.920	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	2832.00		NIST Webbook
tb	868.24	K	Joback Method
tc	1063.09	K	Joback Method
tf	503.53	K	Joback Method
vc	1.371	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1166.36	J/molxK	868.24	Joback Method
cpg	1186.44	J/molxK	900.72	Joback Method
cpg	1205.31	J/molxK	933.19	Joback Method
cpg	1223.00	J/molxK	965.67	Joback Method
cpg	1239.57	J/molxK	998.14	Joback Method
cpg	1255.06	J/molxK	1030.62	Joback Method
cpg	1269.52	J/molxK	1063.09	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=U321568&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321568&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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