

# Sarcosylsarcosine, N-isobutoxycarbonyl-, isoheptyl ester

<b>Inchi:</b>	InChI=1S/C17H32N2O5/c1-13(2)8-7-9-23-16(21)11-18(5)15(20)10-19(6)17(22)24-12-14
<b>InchiKey:</b>	HZZQTEAVDOHYJZ-UHFFFAOYSA-N
<b>Formula:</b>	C17H32N2O5
<b>SMILES:</b>	CC(C)CCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	344.45

## Physical Properties

Property code	Value	Unit	Source
gf	-287.82	kJ/mol	Joback Method
hf	-871.89	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	81.80	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.149		Crippen Method
mcvol	286.800	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	818.81	K	Joback Method
tc	1008.56	K	Joback Method
tf	510.54	K	Joback Method
vc	1.065	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.11	J/mol×K	818.81	Joback Method
cpg	915.22	J/mol×K	850.43	Joback Method
cpg	930.29	J/mol×K	882.06	Joback Method
cpg	944.32	J/mol×K	913.68	Joback Method
cpg	957.34	J/mol×K	945.31	Joback Method
cpg	969.39	J/mol×K	976.93	Joback Method
cpg	980.47	J/mol×K	1008.56	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=U320580&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320580&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>
<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>h vap:</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>r in pol:</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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