

# Sarcosylsarcosine, N-isobutoxycarbonyl-, butyl ester

Inchi:	InChI=1S/C15H28N2O5/c1-6-7-8-21-14(19)10-16(4)13(18)9-17(5)15(20)22-11-12(2)3/h1
InchiKey:	DHFKALVZKRFMAZ-UHFFFAOYSA-N
Formula:	C15H28N2O5
SMILES:	CCCCOC(=O)CN(C)C(=O)CN(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	316.39

## Physical Properties

Property code	Value	Unit	Source
gf	-302.22	kJ/mol	Joback Method
hf	-825.33	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	77.74	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.512		Crippen Method
mvol	258.620	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	773.49	K	Joback Method
tc	958.90	K	Joback Method
tf	503.00	K	Joback Method
vc	0.960	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.31	J/mol×K	773.49	Joback Method
cpg	797.65	J/mol×K	804.39	Joback Method
cpg	812.05	J/mol×K	835.29	Joback Method
cpg	825.55	J/mol×K	866.19	Joback Method
cpg	838.14	J/mol×K	897.09	Joback Method
cpg	849.85	J/mol×K	928.00	Joback Method
cpg	860.71	J/mol×K	958.90	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U320579&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U320579&amp;Units=SI</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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