

# Sarcosine, N-(2-bromobenzoyl)-, butyl ester

<b>Inchi:</b>	InChI=1S/C14H18BrNO3/c1-3-4-9-19-13(17)10-16(2)14(18)11-7-5-6-8-12(11)15/h5-8H,3
<b>InchiKey:</b>	ZTWKAIDGRYRXMZ-UHFFFAOYSA-N
<b>Formula:</b>	C14H18BrNO3
<b>SMILES:</b>	CCCCOC(=O)CN(C)C(=O)c1ccccc1Br
<b>Mol. weight [g/mol]:</b>	328.20

## Physical Properties

Property code	Value	Unit	Source
gf	-67.96	kJ/mol	Joback Method
hf	-370.75	kJ/mol	Joback Method
hfus	38.36	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.864		Crippen Method
mcvol	220.850	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	760.14	K	Joback Method
tc	975.72	K	Joback Method
tf	500.84	K	Joback Method
vc	0.822	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.33	J/molxK	760.14	Joback Method
cpg	604.67	J/molxK	796.07	Joback Method
cpg	617.07	J/molxK	832.00	Joback Method
cpg	628.55	J/molxK	867.93	Joback Method
cpg	639.18	J/molxK	903.86	Joback Method
cpg	648.98	J/molxK	939.79	Joback Method
cpg	658.00	J/molxK	975.72	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321451&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321451&amp;Units=SI</a>
<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.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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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