

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

<b>Inchi:</b>	InChI=1S/C19H28BrNO3/c1-3-4-5-6-7-8-11-14-24-18(22)15-21(2)19(23)16-12-9-10-13-1
<b>InchiKey:</b>	PMHPEJRPTSGYAK-UHFFFAOYSA-N
<b>Formula:</b>	C19H28BrNO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
<b>Mol. weight [g/mol]:</b>	398.33

## Physical Properties

Property code	Value	Unit	Source
gf	-25.86	kJ/mol	Joback Method
hf	-473.95	kJ/mol	Joback Method
hfus	51.31	kJ/mol	Joback Method
hvap	85.21	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.815		Crippen Method
mcvol	291.300	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	874.54	K	Joback Method
tc	1083.90	K	Joback Method
tf	557.19	K	Joback Method
vc	1.101	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.20	J/molxK	874.54	Joback Method
cpg	887.98	J/molxK	909.43	Joback Method
cpg	901.72	J/molxK	944.33	Joback Method
cpg	914.47	J/molxK	979.22	Joback Method
cpg	926.31	J/molxK	1014.11	Joback Method
cpg	937.27	J/molxK	1049.01	Joback Method
cpg	947.41	J/molxK	1083.90	Joback Method

# Sources

<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=U321456&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321456&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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