

# Sarcosine, N-(4-bromobenzoyl)-, decyl ester

<b>Inchi:</b>	InChI=1S/C20H30BrNO3/c1-3-4-5-6-7-8-9-10-15-25-19(23)16-22(2)20(24)17-11-13-18(2)
<b>InchiKey:</b>	YIZZCYNNUNVFZ-UHFFFAOYSA-N
<b>Formula:</b>	C20H30BrNO3
<b>SMILES:</b>	CCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(Br)cc1
<b>Mol. weight [g/mol]:</b>	412.36

## Physical Properties

Property code	Value	Unit	Source
gf	-17.44	kJ/mol	Joback Method
hf	-494.59	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	87.43	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.205		Crippen Method
mcvol	305.390	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinqol	2941.00		NIST Webbook
tb	897.42	K	Joback Method
tc	1107.57	K	Joback Method
tf	568.46	K	Joback Method
vc	1.157	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.14	J/molxK	897.42	Joback Method
cpg	947.17	J/molxK	932.44	Joback Method
cpg	961.14	J/molxK	967.47	Joback Method
cpg	974.11	J/molxK	1002.49	Joback Method
cpg	986.14	J/molxK	1037.52	Joback Method
cpg	997.28	J/molxK	1072.54	Joback Method
cpg	1007.60	J/molxK	1107.57	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=U321381&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321381&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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