

# Sarcosine, N-(4-butylbenzoyl)-, dodecyl ester

<b>Inchi:</b>	InChI=1S/C26H43NO3/c1-4-6-8-9-10-11-12-13-14-15-21-30-25(28)22-27(3)26(29)24-19
<b>InchiKey:</b>	RKKWLSWURKANER-UHFFFAOYSA-N
<b>Formula:</b>	C26H43NO3
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccc(CCCC)cc1
<b>Mol. weight [g/mol]:</b>	417.62

## Physical Properties

Property code	Value	Unit	Source
gf	18.76	kJ/mol	Joback Method
hf	-644.76	kJ/mol	Joback Method
hfus	64.16	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	6.565		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
tb	968.54	K	Joback Method
tc	1186.07	K	Joback Method
tf	576.28	K	Joback Method
vc	1.431	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1257.68	J/molxK	968.54	Joback Method
cpg	1276.04	J/molxK	1004.79	Joback Method
cpg	1293.03	J/molxK	1041.05	Joback Method
cpg	1308.70	J/molxK	1077.30	Joback Method
cpg	1323.15	J/molxK	1113.56	Joback Method
cpg	1336.44	J/molxK	1149.81	Joback Method
cpg	1348.66	J/molxK	1186.07	Joback Method

# Sources

<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>
<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=U321141&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321141&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>hvap:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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