

# Sarcosine, N-(4-nitrobenzoyl)-, heptyl ester

<b>Inchi:</b>	InChI=1S/C17H24N2O5/c1-3-4-5-6-7-12-24-16(20)13-18(2)17(21)14-8-10-15(11-9-14)19
<b>InchiKey:</b>	LQCHYZDWIDKALS-UHFFFAOYSA-N
<b>Formula:</b>	C17H24N2O5
<b>SMILES:</b>	CCCCCCCOC(=O)CN(C)C(=O)c1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	336.38

## Physical Properties

Property code	Value	Unit	Source
gf	-21.47	kJ/mol	Joback Method
hf	-469.76	kJ/mol	Joback Method
hfus	52.21	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.180		Crippen Method
mvol	263.040	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	914.46	K	Joback Method
tc	1135.53	K	Joback Method
tf	618.46	K	Joback Method
vc	1.010	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.31	J/mol×K	914.46	Joback Method
cpg	840.22	J/mol×K	951.31	Joback Method
cpg	852.03	J/mol×K	988.15	Joback Method
cpg	862.80	J/mol×K	1025.00	Joback Method
cpg	872.57	J/mol×K	1061.84	Joback Method
cpg	881.39	J/mol×K	1098.69	Joback Method
cpg	889.33	J/mol×K	1135.53	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=U321286&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321286&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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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