

# «beta»-Alanine, N-acryloyl-, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C20H37NO3/c1-3-5-6-7-8-9-10-11-12-13-14-15-18-24-20(23)16-17-21-19(22)4
<b>InchiKey:</b>	XWOJQYCYIOEHDB-UHFFFAOYSA-N
<b>Formula:</b>	C20H37NO3
<b>SMILES:</b>	C=CC(=O)NCCC(=O)OCCCCCCCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	339.51

## Physical Properties

Property code	Value	Unit	Source
gf	-68.09	kJ/mol	Joback Method
hf	-634.61	kJ/mol	Joback Method
hfus	55.76	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.923		Crippen Method
mcvol	307.350	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	2607.00		NIST Webbook
tb	834.01	K	Joback Method
tc	1022.91	K	Joback Method
tf	488.15	K	Joback Method
vc	1.202	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.72	J/molxK	834.01	Joback Method
cpg	992.25	J/molxK	865.49	Joback Method
cpg	1008.76	J/molxK	896.98	Joback Method
cpg	1024.29	J/molxK	928.46	Joback Method
cpg	1038.85	J/molxK	959.94	Joback Method
cpg	1052.50	J/molxK	991.43	Joback Method
cpg	1065.27	J/molxK	1022.91	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321683&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.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>

# 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>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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