

# «beta»-Alanine, N-(3-methylbenzoyl)-, heptyl ester

Inchi:	InChI=1S/C18H27NO3/c1-3-4-5-6-7-13-22-17(20)11-12-19-18(21)16-10-8-9-15(2)14-16/
InchiKey:	XHGZIJDGLWATJK-UHFFFAOYSA-N
Formula:	C18H27NO3
SMILES:	CCCCCCCOC(=O)CCNC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	305.41

## Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-493.70	kJ/mol	Joback Method
hfus	45.51	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.629		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	823.23	K	Joback Method
tc	1025.77	K	Joback Method
tf	506.31	K	Joback Method
vc	1.000	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.71	J/molxK	823.23	Joback Method
cpg	806.04	J/molxK	856.99	Joback Method
cpg	820.33	J/molxK	890.74	Joback Method
cpg	833.61	J/molxK	924.50	Joback Method
cpg	845.91	J/molxK	958.26	Joback Method
cpg	857.27	J/molxK	992.01	Joback Method
cpg	867.73	J/molxK	1025.77	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=U321630&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321630&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>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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