

# «beta»-Alanine, N-isobutyryl-, octadecyl ester

<b>Inchi:</b>	InChI=1S/C25H49NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-29-24(27)20-2
<b>InchiKey:</b>	ZXNDCWQUKBGJPR-UHFFFAOYSA-N
<b>Formula:</b>	C25H49NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)CCNC(=O)C(C)C
<b>Mol. weight [g/mol]:</b>	411.66

## Physical Properties

Property code	Value	Unit	Source
gf	-116.27	kJ/mol	Joback Method
hf	-868.52	kJ/mol	Joback Method
hfus	66.47	kJ/mol	Joback Method
hvap	93.19	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.953		Crippen Method
mvol	382.100	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rmpol	3166.00		NIST Webbook
tb	951.29	K	Joback Method
tc	1169.40	K	Joback Method
tf	531.26	K	Joback Method
vc	1.494	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.74	J/mol×K	951.29	Joback Method
cpg	1336.40	J/mol×K	987.64	Joback Method
cpg	1355.53	J/mol×K	1023.99	Joback Method
cpg	1373.20	J/mol×K	1060.34	Joback Method
cpg	1389.47	J/mol×K	1096.69	Joback Method
cpg	1404.41	J/mol×K	1133.04	Joback Method
cpg	1418.08	J/mol×K	1169.40	Joback Method

# Sources

<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=U321675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321675&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>
<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>

# 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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