

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

Inchi:	InChI=1S/C22H43NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-26-21(24)17-18-23-22(2
InchiKey:	WYXNMQPJPFDDGB-UHFFFAOYSA-N
Formula:	C22H43NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)C(C)C
Mol. weight [g/mol]:	369.58

## Physical Properties

Property code	Value	Unit	Source
gf	-141.53	kJ/mol	Joback Method
hf	-806.60	kJ/mol	Joback Method
hfus	58.70	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.783		Crippen Method
mcvol	339.830	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2723.00		NIST Webbook
tb	882.65	K	Joback Method
tc	1080.61	K	Joback Method
tf	497.45	K	Joback Method
vc	1.327	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.11	J/molxK	882.65	Joback Method
cpg	1145.13	J/molxK	915.64	Joback Method
cpg	1162.92	J/molxK	948.64	Joback Method
cpg	1179.54	J/molxK	981.63	Joback Method
cpg	1195.02	J/molxK	1014.62	Joback Method
cpg	1209.40	J/molxK	1047.62	Joback Method
cpg	1222.71	J/molxK	1080.61	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=U321672&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321672&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>

# 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>hvac:</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>mccol:</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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