

# «gamma»-Aminobutyric acid, N-isobutoxycarbonyl-, isobutyl ester

**Other names:** .gama.-Aminobutyric acid, N-isobutoxycarbonyl-, isobutyl ester

**Inchi:** InChI=1S/C13H25NO4/c1-10(2)8-17-12(15)6-5-7-14-13(16)18-9-11(3)4/h10-11H,5-9H2,1

**InchiKey:** NTZXMVBZERHXOP-UHFFFAOYSA-N

**Formula:** C13H25NO4

**SMILES:** CC(C)COC(=O)CCCNC(=O)OCC(C)C

**Mol. weight [g/mol]:** 259.34

## Physical Properties

Property code	Value	Unit	Source
gf	-324.75	kJ/mol	Joback Method
hf	-758.34	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.348		Crippen Method
mvol	218.890	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1834.00		NIST Webbook
tb	698.71	K	Joback Method
tc	882.99	K	Joback Method
tf	403.25	K	Joback Method
vc	0.835	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.67	J/mol×K	698.71	Joback Method
cpg	642.00	J/mol×K	729.42	Joback Method
cpg	656.53	J/mol×K	760.14	Joback Method
cpg	670.26	J/mol×K	790.85	Joback Method
cpg	683.21	J/mol×K	821.56	Joback Method
cpg	695.37	J/mol×K	852.27	Joback Method
cpg	706.75	J/mol×K	882.99	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321046&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321046&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>hvp:</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>rinp:</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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