

# Glutamic acid, n-[(2-chloroethyl)carbamoyl]-, dimethyl ester

Inchi:	InChI=1S/C10H17ClN2O5/c1-17-8(14)4-3-7(9(15)18-2)13-10(16)12-6-5-11/h7H,3-6H2,1-
InchiKey:	GPIOBGGCQVFDRC-UHFFFAOYSA-N
Formula:	C10H17ClN2O5
SMILES:	COC(=O)CCC(NC(=O)NCCCl)C(=O)OC
Mol. weight [g/mol]:	280.70
CAS:	13908-06-0

## Physical Properties

Property code	Value	Unit	Source
gf	-399.03	kJ/mol	Joback Method
hf	-765.99	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	0.019		Crippen Method
mcvol	200.410	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	771.98	K	Joback Method
tc	970.16	K	Joback Method
tf	516.95	K	Joback Method
vc	0.762	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.03	J/molxK	771.98	Joback Method
cpg	572.18	J/molxK	805.01	Joback Method
cpg	582.53	J/molxK	838.04	Joback Method
cpg	592.09	J/molxK	871.07	Joback Method
cpg	600.87	J/molxK	904.10	Joback Method
cpg	608.86	J/molxK	937.13	Joback Method
cpg	616.06	J/molxK	970.16	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=C13908060&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908060&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>

# 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>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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