

# (Beta-cyclopropyl)-alanine

<b>Inchi:</b>	InChI=1S/C6H11NO2/c7-5(6(8)9)3-4-1-2-4/h4-5H,1-3,7H2,(H,8,9)
<b>InchiKey:</b>	XGUXJMWPVJQIHI-UHFFFAOYSA-N
<b>Formula:</b>	C6H11NO2
<b>SMILES:</b>	NC(CC1CC1)C(=O)O
<b>Mol. weight [g/mol]:</b>	129.16
<b>CAS:</b>	15785-52-1

## Physical Properties

Property code	Value	Unit	Source
gf	-141.34	kJ/mol	Joback Method
hf	-330.67	kJ/mol	Joback Method
hfus	16.79	kJ/mol	Joback Method
hvap	62.54	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.198		Crippen Method
mcvol	101.960	ml/mol	McGowan Method
pc	4795.85	kPa	Joback Method
tb	561.56	K	Joback Method
tc	759.70	K	Joback Method
tf	354.33	K	Joback Method
vc	0.377	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.05	J/molxK	561.56	Joback Method
cpg	269.88	J/molxK	594.58	Joback Method
cpg	279.12	J/molxK	627.61	Joback Method
cpg	287.79	J/molxK	660.63	Joback Method
cpg	295.93	J/molxK	693.65	Joback Method
cpg	303.57	J/molxK	726.68	Joback Method
cpg	310.76	J/molxK	759.70	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=C15785521&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15785521&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>
<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>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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