

# (S)-(+)-2-(Methoxymethyl)pyrrolidine

<b>Inchi:</b>	InChI=1S/C6H13NO/c1-8-5-6-3-2-4-7-6/h6-7H,2-5H2,1H3/t6-/m1/s1
<b>InchiKey:</b>	CHPRFKYDQRKRRK-ZCFIWIBFSA-N
<b>Formula:</b>	C6H13NO
<b>SMILES:</b>	COCC1CCCN1
<b>Mol. weight [g/mol]:</b>	115.17
<b>CAS:</b>	63126-47-6

## Physical Properties

Property code	Value	Unit	Source
gf	18.90	kJ/mol	Joback Method
hf	-201.10	kJ/mol	Joback Method
hfus	16.01	kJ/mol	Joback Method
hvap	38.38	kJ/mol	Joback Method
log10ws	-0.62		Crippen Method
logp	0.385		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	422.93	K	Joback Method
tc	627.21	K	Joback Method
tf	295.54	K	Joback Method
vc	0.367	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.05	J/molxK	422.93	Joback Method
cpg	213.96	J/molxK	456.98	Joback Method
cpg	227.31	J/molxK	491.02	Joback Method
cpg	240.10	J/molxK	525.07	Joback Method
cpg	252.33	J/molxK	559.12	Joback Method
cpg	264.01	J/molxK	593.17	Joback Method
cpg	275.15	J/molxK	627.21	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	5.30	NIST Webbook

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C63126476&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63126476&amp;Units=SI</a>
Crippen Method:	<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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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