

# (S)-(+)-Isoleucinol

<b>Other names:</b>	1-Pentanol, 2-amino-3-methyl-, [S-(R*,R*)]- 2-amino-3-methylpentan-1-ol
<b>Inchi:</b>	InChI=1S/C6H15NO/c1-3-5(2)6(7)4-8/h5-6,8H,3-4,7H2,1-2H3
<b>InchiKey:</b>	VTQHAQXFSDMHT-UHFFFAOYSA-N
<b>Formula:</b>	C6H15NO
<b>SMILES:</b>	CCC(C)C(N)CO
<b>Mol. weight [g/mol]:</b>	117.19
<b>CAS:</b>	24629-25-2

## Physical Properties

Property code	Value	Unit	Source
gf	-75.61	kJ/mol	Joback Method
hf	-296.17	kJ/mol	Joback Method
hfus	13.53	kJ/mol	Joback Method
hvap	55.49	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.352		Crippen Method
mvol	111.250	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	500.51	K	Joback Method
tc	680.59	K	Joback Method
tf	271.46	K	Joback Method
vc	0.407	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.10	J/molxK	500.51	Joback Method
cpg	271.63	J/molxK	530.52	Joback Method
cpg	281.69	J/molxK	560.54	Joback Method
cpg	291.31	J/molxK	590.55	Joback Method
cpg	300.49	J/molxK	620.56	Joback Method
cpg	309.25	J/molxK	650.57	Joback Method
cpg	317.61	J/molxK	680.59	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.20	K	1.90	NIST Webbook

## Sources

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=C24629252&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C24629252&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>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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