

# Muurool-5-en-4-one <cis-14-nor->

<b>Inchi:</b>	InChI=1S/C14H22O/c1-9(2)12-6-4-10(3)13-7-5-11(15)8-14(12)13/h8-10,12-13H,4-7H2,1
<b>InchiKey:</b>	AQNMVDGKNNYA EW-UHFFFAOYSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC(C)C1CCC(C)C2CCC(=O)C=C12
<b>Mol. weight [g/mol]:</b>	206.32
<b>CAS:</b>	63180-33-6

## Physical Properties

Property code	Value	Unit	Source
gf	27.69	kJ/mol	Joback Method
hf	-328.34	kJ/mol	Joback Method
hfus	17.78	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.594		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	1689.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1696.30		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1696.30		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	617.13	K	Joback Method
tc	846.53	K	Joback Method
tf	331.60	K	Joback Method
vc	0.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.90	J/mol×K	617.13	Joback Method
cpg	534.67	J/mol×K	655.36	Joback Method
cpg	556.06	J/mol×K	693.60	Joback Method

cpg	576.08	J/mol×K	731.83	Joback Method
cpg	594.76	J/mol×K	770.06	Joback Method
cpg	612.12	J/mol×K	808.30	Joback Method
cpg	628.19	J/mol×K	846.53	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C63180336&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63180336&amp;Units=SI</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>rinpola:</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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