

# 13-nor-Eudesm-5-en-11-one, 7«alpha»

<b>Inchi:</b>	InChI=1S/C14H22O/c1-10-5-4-7-14(3)8-6-12(11(2)15)9-13(10)14/h9-10,12H,4-8H2,1-3H
<b>InchiKey:</b>	SEPLFXIHUVTSIX-ZKYQVNSYSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC(=O)C1C=C2C(C)CCCC2(C)CC1
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	18.31	kJ/mol	Joback Method
hf	-282.70	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1540.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	603.86	K	Joback Method
tc	831.60	K	Joback Method
tf	352.21	K	Joback Method
vc	0.691	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.13	J/molxK	603.86	Joback Method
cpg	518.51	J/molxK	641.82	Joback Method
cpg	538.57	J/molxK	679.77	Joback Method
cpg	557.47	J/molxK	717.73	Joback Method
cpg	575.36	J/molxK	755.68	Joback Method
cpg	592.39	J/molxK	793.64	Joback Method
cpg	608.73	J/molxK	831.60	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=R397796&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R397796&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>

# 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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