

# (+)-(1S,3aR,7S,7aR)-2,3,3a,4,5,6,7,7a-Octahydro-7,

<b>Inchi:</b>	InChI=1S/C15H26O/c1-10(2)14(16)13-9-8-12-7-5-6-11(3)15(12,13)4/h10-13H,5-9H2,1-4
<b>InchiKey:</b>	VLBHRLBDSSUVAV-UKTARXLSSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC(C)C(=O)C1CCC2CCCC(C)C21C
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	8.35	kJ/mol	Joback Method
hf	-369.11	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	53.91	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinsol	1601.00		NIST Webbook
rinsol	1601.00		NIST Webbook
tb	613.22	K	Joback Method
tc	831.03	K	Joback Method
tf	334.48	K	Joback Method
vc	0.761	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.80	J/molxK	613.22	Joback Method
cpg	593.78	J/molxK	649.52	Joback Method
cpg	615.41	J/molxK	685.82	Joback Method
cpg	635.85	J/molxK	722.13	Joback Method
cpg	655.24	J/molxK	758.43	Joback Method
cpg	673.72	J/molxK	794.73	Joback Method
cpg	691.44	J/molxK	831.03	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=R281562&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R281562&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>hvp:</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>rinp:</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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