

# (+)-(5S,10S)-Eudesma-3,7(11)-dien-8-one

<b>Inchi:</b>	InChI=1S/C15H22O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)9-14(12)16/h6,13H,5,7-9H2,1-4
<b>InchiKey:</b>	LLUFBBLIDQULSW-ZFWWWQNUSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC1=CCCC2(C)CC(=O)C(=C(C)C)CC12
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	77.68	kJ/mol	Joback Method
hf	-241.88	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	54.42	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinsol	1745.00		NIST Webbook
tb	651.88	K	Joback Method
tc	891.67	K	Joback Method
tf	382.41	K	Joback Method
vc	0.733	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.30	J/mol×K	651.88	Joback Method
cpg	560.66	J/mol×K	691.85	Joback Method
cpg	580.83	J/mol×K	731.81	Joback Method
cpg	599.99	J/mol×K	771.78	Joback Method
cpg	618.29	J/mol×K	811.74	Joback Method
cpg	635.88	J/mol×K	851.71	Joback Method
cpg	652.93	J/mol×K	891.67	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=R561398&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R561398&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>rinpol:</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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