

# (-)-(5R,7R,10S)-eudesm-4(15)-en-6-one

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10(2)12-7-9-15(4)8-5-6-11(3)13(15)14(12)16/h10,12-13H,3,5-9H
<b>InchiKey:</b>	TYQALBNCJWAILN-YOYPFHDYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCCC2(C)CCC(C(C)C)C(=O)C12</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	63.37	kJ/mol	Joback Method
hf	-295.81	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1617.00		NIST Webbook
tb	635.27	K	Joback Method
tc	867.84	K	Joback Method
tf	367.17	K	Joback Method
vc	0.740	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.21	J/mol×K	635.27	Joback Method
cpg	585.42	J/mol×K	674.03	Joback Method
cpg	607.31	J/mol×K	712.79	Joback Method
cpg	628.03	J/mol×K	751.56	Joback Method
cpg	647.71	J/mol×K	790.32	Joback Method
cpg	666.46	J/mol×K	829.08	Joback Method
cpg	684.43	J/mol×K	867.84	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=R422872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R422872&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.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>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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