

# (1S,4aR,7R)-1,4a-Dimethyl-7-(prop-1-en-2-yl)-1,2,3

<b>Inchi:</b>	InChI=1S/C15H24/c1-11(2)13-7-9-15(4)8-5-6-12(3)14(15)10-13/h10,12-13H,1,5-9H2,2-4
<b>InchiKey:</b>	MZWGOWHEHPSPES-UHFFFAOYSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C(C)C1C=C2C(C)CCCC2(C)CC1</chem>
<b>Mol. weight [g/mol]:</b>	204.35
<b>CAS:</b>	52026-55-8

## Physical Properties

Property code	Value	Unit	Source
gf	234.94	kJ/mol	Joback Method
hf	-75.12	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1446.50		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1620.00		NIST Webbook
tb	569.43	K	Joback Method
tc	794.31	K	Joback Method
tf	297.83	K	Joback Method
vc	0.723	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.65	J/molxK	569.43	Joback Method
cpg	523.17	J/molxK	606.91	Joback Method
cpg	545.19	J/molxK	644.39	Joback Method
cpg	565.88	J/molxK	681.87	Joback Method
cpg	585.40	J/molxK	719.35	Joback Method
cpg	603.90	J/molxK	756.83	Joback Method

## Sources

<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=C52026558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52026558&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>

## 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>ripol:</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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