

# 2-Methyltridec-2-en-4-one

<b>Inchi:</b>	InChI=1S/C14H26O/c1-4-5-6-7-8-9-10-11-14(15)12-13(2)3/h12H,4-11H2,1-3H3
<b>InchiKey:</b>	MHMPYFBKZUSOQX-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O
<b>SMILES:</b>	CCCCCCCCC(=O)C=C(C)C
<b>Mol. weight [g/mol]:</b>	210.36

## Physical Properties

Property code	Value	Unit	Source
gf	9.75	kJ/mol	Joback Method
hf	-337.44	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.662		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinsol	1593.00		NIST Webbook
tb	577.63	K	Joback Method
tc	754.53	K	Joback Method
tf	278.43	K	Joback Method
vc	0.806	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.48	J/mol×K	577.63	Joback Method
cpg	535.51	J/mol×K	607.11	Joback Method
cpg	551.76	J/mol×K	636.60	Joback Method
cpg	567.26	J/mol×K	666.08	Joback Method
cpg	582.05	J/mol×K	695.56	Joback Method
cpg	596.14	J/mol×K	725.05	Joback Method
cpg	609.57	J/mol×K	754.53	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R508842&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R508842&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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