

# 9-Undecenal, 2,6,10-trimethyl-

<b>Other names:</b>	2,6,10-Trimethyl-9-undecen-1-al 2,6,10-Trimethyl-9-undecenal 2,6,10-trimethylundec-9-enal Adoxal
<b>Inchi:</b>	InChI=1S/C14H26O/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15/h7,11,13-14H,5-6,8-10H2,1-4
<b>InchiKey:</b>	UEGBWDUVDAKUGA-UHFFFAOYSA-N
<b>Formula:</b>	C14H26O
<b>SMILES:</b>	CC(C)=CCCC(C)CCCC(C)C=O
<b>Mol. weight [g/mol]:</b>	210.36
<b>CAS:</b>	141-13-9

## Physical Properties

Property code	Value	Unit	Source
gf	34.27	kJ/mol	Joback Method
hf	-321.00	kJ/mol	Joback Method
hfus	26.15	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.374		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1387.00		NIST Webbook
tb	571.54	K	Joback Method
tc	751.07	K	Joback Method
tf	240.50	K	Joback Method
vc	0.805	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.92	J/molxK	571.54	Joback Method
cpg	536.34	J/molxK	601.46	Joback Method

cpg	552.94	J/mol×K	631.38	Joback Method
cpg	568.75	J/mol×K	661.30	Joback Method
cpg	583.80	J/mol×K	691.23	Joback Method
cpg	598.13	J/mol×K	721.15	Joback Method
cpg	611.76	J/mol×K	751.07	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.36509e+01
Coeff. B	-4.32368e+03
Coeff. C	-9.43700e+01
Temperature range (K), min.	417.92
Temperature range (K), max.	612.84

## Sources

<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C141139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C141139&amp;Units=SI</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>pvap:</b>	Vapor 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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