

# 2,6,10-Dodecatrienal, 3,7,11-trimethyl-, (Z,E)-

<b>Other names:</b>	cis, trans-Farnesal 2-cis-6-trans-Farnesal (2Z,6E)-3,7,11-Trimethyl-2,6,10-dodecatrienal Z,E-Farnesal (2Z,6E)-Farnesal
<b>Inchi:</b>	InChI=1S/C15H24O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h7,9,11-12H,5-6,8,10H2,1
<b>InchiKey:</b>	YHRUHBBTQZKMEX-PVMFERMNSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)=CCCC(C)=CCCC(C)=CC=O
<b>Mol. weight [g/mol]:</b>	220.35
<b>CAS:</b>	4380-32-9

## Physical Properties

Property code	Value	Unit	Source
gf	190.91	kJ/mol	Joback Method
hf	-116.22	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	55.82	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.605		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1664.90		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
ripol	2219.00		NIST Webbook
ripol	2219.00		NIST Webbook
tb	603.38	K	Joback Method
tc	794.15	K	Joback Method
tf	243.69	K	Joback Method
vc	0.836	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.64	J/mol×K	603.38	Joback Method
cpg	547.51	J/mol×K	635.18	Joback Method
cpg	563.47	J/mol×K	666.97	Joback Method
cpg	578.59	J/mol×K	698.77	Joback Method
cpg	592.93	J/mol×K	730.56	Joback Method
cpg	606.55	J/mol×K	762.36	Joback Method
cpg	619.50	J/mol×K	794.15	Joback Method

## Sources

<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=C4380329&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4380329&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>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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