

# (E,E,E)-2,4,7-tridecatrienal

Inchi:	InChI=1S/C13H20O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h6-7,9-13H,2-5,8H2,1H3/b7-6+,1-2,3-4,5-6
InchiKey:	BIXIZZVISIZZDM-NRSJTBBXSA-N
Formula:	C13H20O
SMILES:	CCCCC=CCC=CC=CC=O
Mol. weight [g/mol]:	192.30

## Physical Properties

Property code	Value	Unit	Source
gf	199.72	kJ/mol	Joback Method
hf	-45.57	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.824		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinpol	1647.00		NIST Webbook
tb	557.98	K	Joback Method
tc	744.04	K	Joback Method
tf	263.03	K	Joback Method
vc	0.721	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.82	J/molxK	557.98	Joback Method
cpg	445.98	J/molxK	588.99	Joback Method
cpg	460.33	J/molxK	620.00	Joback Method
cpg	473.90	J/molxK	651.01	Joback Method
cpg	486.76	J/molxK	682.02	Joback Method
cpg	498.94	J/molxK	713.03	Joback Method
cpg	510.51	J/molxK	744.04	Joback Method
dvisc	0.0039796	Paxs	263.03	Joback Method
dvisc	0.0014768	Paxs	312.19	Joback Method

dvisc	0.0007177	Paxs	361.35	Joback Method
dvisc	0.0004146	Paxs	410.50	Joback Method
dvisc	0.0002693	Paxs	459.66	Joback Method
dvisc	0.0001902	Paxs	508.82	Joback Method
dvisc	0.0001428	Paxs	557.98	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=R237040&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R237040&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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