

# Megastigma-4,6(Z),8(E)-triene

<b>Other names:</b>	Cyclohexene, 6-(2-butenylidene)-1,5,5-trimethyl-, (Z,E)- Cyclohexene, 6-(2E)-2-buten-1-ylidene-1,5,5-trimethyl-, (6Z)-
<b>Inchi:</b>	InChI=1S/C13H20/c1-5-6-9-12-11(2)8-7-10-13(12,3)4/h5-6,8-9H,7,10H2,1-4H3/b6-5+,12
<b>InchiKey:</b>	BYDQKMZEOZVIJM-HFACTSAFSA-N
<b>Formula:</b>	C13H20
<b>SMILES:</b>	CC=CC=C1C(C)=CCCC1(C)C
<b>Mol. weight [g/mol]:</b>	176.30
<b>CAS:</b>	51468-85-0

## Physical Properties

Property code	Value	Unit	Source
gf	223.55	kJ/mol	Joback Method
hf	-2.53	kJ/mol	Joback Method
hfus	16.32	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1351.00		NIST Webbook
ripol	2323.00		NIST Webbook
ripol	2323.00		NIST Webbook
tb	531.57	K	Joback Method
tc	748.41	K	Joback Method
tf	286.11	K	Joback Method
vc	0.643	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.30	J/molxK	531.57	Joback Method
cpg	413.03	J/molxK	567.71	Joback Method

cpg	430.58	J/mol×K	603.85	Joback Method
cpg	447.07	J/mol×K	639.99	Joback Method
cpg	462.65	J/mol×K	676.13	Joback Method
cpg	477.45	J/mol×K	712.27	Joback Method
cpg	491.60	J/mol×K	748.41	Joback Method

## Sources

<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=C51468850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51468850&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>

## 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>rinpola:</b>	Non-polar retention indices
<b>ripola:</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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