

# (E,E)-2,5-Epoxy-6,8-megastigmadiene

<b>Inchi:</b>	InChI=1S/C13H20O/c1-5-6-7-10-12(2,3)11-8-9-13(10,4)14-11/h5-7,11H,8-9H2,1-4H3/b6-
<b>InchiKey:</b>	RRUCICKXWFEVIP-NMVVBPQGSA-N
<b>Formula:</b>	C13H20O
<b>SMILES:</b>	CC=CC=C1C2(C)CCC(O2)C1(C)C
<b>Mol. weight [g/mol]:</b>	192.30

## Physical Properties

Property code	Value	Unit	Source
gf	188.85	kJ/mol	Joback Method
hf	-100.82	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	47.17	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.466		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinpol	1341.00		NIST Webbook
rinpol	1341.00		NIST Webbook
tb	548.15	K	Joback Method
tc	769.15	K	Joback Method
tf	344.04	K	Joback Method
vc	0.648	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.03	J/mol×K	548.15	Joback Method
cpg	448.63	J/mol×K	584.98	Joback Method
cpg	465.85	J/mol×K	621.82	Joback Method
cpg	481.96	J/mol×K	658.65	Joback Method
cpg	497.23	J/mol×K	695.48	Joback Method
cpg	511.93	J/mol×K	732.32	Joback Method
cpg	526.36	J/mol×K	769.15	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R617164&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R617164&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>hvp:</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>rinp:</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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