

# 4,6,8-Megastigmatrien-3-one, isomer # 1

<b>Inchi:</b>	InChI=1S/C13H18O/c1-5-6-7-12-10(2)8-11(14)9-13(12,3)4/h5-8H,9H2,1-4H3/b6-5?,12-7
<b>InchiKey:</b>	CBQXHTWJSZXYSK-DOHVUMKLSA-N
<b>Formula:</b>	C13H18O
<b>SMILES:</b>	CC=CC=C1C(C)=CC(=O)CC1(C)C
<b>Mol. weight [g/mol]:</b>	190.28

## Physical Properties

Property code	Value	Unit	Source
gf	100.96	kJ/mol	Joback Method
hf	-140.23	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.434		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinsol	1585.00		NIST Webbook
tb	599.39	K	Joback Method
tc	830.25	K	Joback Method
tf	354.33	K	Joback Method
vc	0.650	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.35	J/mol×K	599.39	Joback Method
cpg	445.16	J/mol×K	637.87	Joback Method
cpg	462.00	J/mol×K	676.34	Joback Method
cpg	478.00	J/mol×K	714.82	Joback Method
cpg	493.28	J/mol×K	753.29	Joback Method
cpg	507.98	J/mol×K	791.77	Joback Method
cpg	522.21	J/mol×K	830.25	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=R591092&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591092&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>mccvol:</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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