

# Megastigma-6(E),8(Z)-dien-4-one

<b>Inchi:</b>	InChI=1S/C13H20O/c1-5-6-7-11-10(2)12(14)8-9-13(11,3)4/h5-7,10H,8-9H2,1-4H3/b6-5-
<b>InchiKey:</b>	YYXHVEGUQLRLSY-GNLLZQBYS-A-N
<b>Formula:</b>	C13H20O
<b>SMILES:</b>	CC=CC=C1C(C)C(=O)CCC1(C)C
<b>Mol. weight [g/mol]:</b>	192.30

## Physical Properties

Property code	Value	Unit	Source
gf	72.92	kJ/mol	Joback Method
hf	-206.88	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	48.49	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.514		Crippen Method
mvol	176.140	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook
tb	590.58	K	Joback Method
tc	818.25	K	Joback Method
tf	336.81	K	Joback Method
vc	0.663	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.51	J/mol×K	590.58	Joback Method
cpg	469.24	J/mol×K	628.53	Joback Method
cpg	487.90	J/mol×K	666.47	Joback Method
cpg	505.59	J/mol×K	704.42	Joback Method
cpg	522.44	J/mol×K	742.36	Joback Method
cpg	538.57	J/mol×K	780.31	Joback Method
cpg	554.08	J/mol×K	818.25	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.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=R493686&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R493686&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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