

# (E,E,E)-1,5,9-Cyclododecatriene, 3-methyl

Inchi:	InChI=1S/C13H20/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h2-3,8-11,13H,4-7,12H2,1H3/b3-2
InchiKey:	OQDOPRBIHXJP-PVXCSLJCSA-N
Formula:	C13H20
SMILES:	CC1C=CCCC=CCCC=CC1
Mol. weight [g/mol]:	176.30

## Physical Properties

Property code	Value	Unit	Source
gf	100.31	kJ/mol	Joback Method
hf	-120.95	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinsol	1308.00		NIST Webbook
tb	539.49	K	Joback Method
tc	782.60	K	Joback Method
tf	224.81	K	Joback Method
vc	0.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.08	J/molxK	539.49	Joback Method
cpg	508.36	J/molxK	742.08	Joback Method
cpg	489.42	J/molxK	701.56	Joback Method
cpg	468.92	J/molxK	661.04	Joback Method
cpg	446.86	J/molxK	620.53	Joback Method
cpg	423.24	J/molxK	580.01	Joback Method
cpg	525.73	J/molxK	782.60	Joback Method
dvisc	0.0000563	Paxs	539.49	Joback Method
dvisc	0.0000956	Paxs	487.04	Joback Method

dvisc	0.0001844	Paxs	434.60	Joback Method
dvisc	0.0004261	Paxs	382.15	Joback Method
dvisc	0.0012850	Paxs	329.70	Joback Method
dvisc	0.0058834	Paxs	277.26	Joback Method
dvisc	0.0547834	Paxs	224.81	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=R2765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R2765&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>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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