

# Thujopsadiene

<b>Inchi:</b>	InChI=1S/C15H22/c1-11-6-9-14(4)8-5-7-13(2,3)15(14)10-12(11)15/h5-7,12H,8-10H2,1-4
<b>InchiKey:</b>	HIRCZOSUMSSTDU-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	CC1=CCC2(C)CC=CC(C)(C)C23CC13
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	259.58	kJ/mol	Joback Method
hf	-17.38	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1445.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1460.00		NIST Webbook
ripol	1650.00		NIST Webbook
tb	570.71	K	Joback Method
tc	808.01	K	Joback Method
tf	387.09	K	Joback Method
vc	0.696	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.77	J/molxK	570.71	Joback Method

cpg	502.91	J/mol×K	610.26	Joback Method
cpg	522.45	J/mol×K	649.81	Joback Method
cpg	540.85	J/mol×K	689.36	Joback Method
cpg	558.58	J/mol×K	728.91	Joback Method
cpg	576.10	J/mol×K	768.46	Joback Method
cpg	593.88	J/mol×K	808.01	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=R224549&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R224549&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Non-polar retention indices
<b>ripol:</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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