

# trans-Thujene

<b>Inchi:</b>	InChI=1S/C10H16/c1-7(2)10-5-4-8(3)9(10)6-10/h4,7,9H,5-6H2,1-3H3/t9-,10-/m0/s1
<b>InchiKey:</b>	KQAZVFVVOEIRWHN-UWVGGRQHSA-N
<b>Formula:</b>	C10H16
<b>SMILES:</b>	CC1=CCC2(C(C)C)CC12
<b>Mol. weight [g/mol]:</b>	136.23

## Physical Properties

Property code	Value	Unit	Source
gf	167.22	kJ/mol	Joback Method
hf	-47.86	kJ/mol	Joback Method
hfus	8.94	kJ/mol	Joback Method
hvap	37.09	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
tb	445.62	K	Joback Method
tc	651.82	K	Joback Method
tf	260.52	K	Joback Method
vc	0.487	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.80	J/mol×K	445.62	Joback Method
cpg	292.04	J/mol×K	479.99	Joback Method
cpg	307.91	J/mol×K	514.35	Joback Method
cpg	322.57	J/mol×K	548.72	Joback Method
cpg	336.15	J/mol×K	583.09	Joback Method
cpg	348.79	J/mol×K	617.45	Joback Method
cpg	360.63	J/mol×K	651.82	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=R407675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R407675&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>rinpola:</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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