

# (E)-Sesquithujen-12-ol

<b>Other names:</b>	(E)-Sesquithujene-12-ol
<b>Inchi:</b>	InChI=1S/C15H24O/c1-11(10-16)5-4-6-13(3)15-8-7-12(2)14(15)9-15/h5,7,13-14,16H,4,6
<b>InchiKey:</b>	ASCIVPSLEDFVHI-BFONTGBQSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(=CCCC(C)C12CC=C(C)C1C2)CO
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	144.17	kJ/mol	Joback Method
hf	-195.86	kJ/mol	Joback Method
hfus	24.87	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1665.00		NIST Webbook
tb	656.24	K	Joback Method
tc	849.04	K	Joback Method
tf	358.65	K	Joback Method
vc	0.767	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.25	J/molxK	656.24	Joback Method
cpg	578.04	J/molxK	688.37	Joback Method
cpg	593.09	J/molxK	720.51	Joback Method
cpg	607.55	J/molxK	752.64	Joback Method
cpg	621.55	J/molxK	784.78	Joback Method
cpg	635.23	J/molxK	816.91	Joback Method
cpg	648.74	J/molxK	849.04	Joback Method

# Sources

<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=R203859&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R203859&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>
<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>

# 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>h vap:</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>r in pol:</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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