

# (E)-sesquithujen-12-al

<b>Inchi:</b>	InChI=1S/C15H22O/c1-11(10-16)5-4-6-13(3)15-8-7-12(2)14(15)9-15/h5,7,10,13-14H,4,6
<b>InchiKey:</b>	XKPPRLYPVCYPRO-BFONTGBQSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC(C=O)=CCCC(C)C12CC=C(C)C1C2
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	181.47	kJ/mol	Joback Method
hf	-129.21	kJ/mol	Joback Method
hfus	23.07	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mvol	193.460	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
tb	612.72	K	Joback Method
tc	820.47	K	Joback Method
tf	339.83	K	Joback Method
vc	0.765	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.40	J/molxK	612.72	Joback Method
cpg	537.77	J/molxK	647.34	Joback Method
cpg	554.10	J/molxK	681.97	Joback Method
cpg	569.59	J/molxK	716.59	Joback Method
cpg	584.39	J/molxK	751.22	Joback Method
cpg	598.68	J/molxK	785.84	Joback Method
cpg	612.63	J/molxK	820.47	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=R233602&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233602&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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