

# Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-

<b>Other names:</b>	(-)-.alpha.-curcumene (-)-ar-curcumene (-)-curcumene (R)-1-methyl-4-(6-methylhept-5-en-2-yl)benzene 1-((1R)-1,5-dimethyl-4-hexenyl)-4-methylbenzene 2-Heptene, 2-methyl-6-p-tolyl- Ar-Curcumene Curcumene «alpha»-Curcumene
<b>Inchi:</b>	InChI=1S/C15H22/c1-12(2)6-5-7-14(4)15-10-8-13(3)9-11-15/h6,8-11,14H,5,7H2,1-4H3
<b>InchiKey:</b>	VMYXUZSZMNBRCN-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	CC(C)=CCCC(C)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	202.34
<b>CAS:</b>	644-30-4

## Physical Properties

Property code	Value	Unit	Source
gf	247.43	kJ/mol	Joback Method
hf	-25.72	kJ/mol	Joback Method
hfus	23.63	kJ/mol	Joback Method
hvap	51.57	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.845		Crippen Method
mcvol	194.150	ml/mol	McGowan Method
pc	1928.74	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1475.00		NIST Webbook
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ripol	1770.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1798.00		NIST Webbook
ripol	1787.50		NIST Webbook
tb	577.86	K	Joback Method
tc	786.13	K	Joback Method
tf	263.71	K	Joback Method
vc	0.743	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.13	J/mol×K	577.86	Joback Method
cpg	492.87	J/mol×K	612.57	Joback Method
cpg	510.53	J/mol×K	647.28	Joback Method
cpg	527.17	J/mol×K	682.00	Joback Method
cpg	542.83	J/mol×K	716.71	Joback Method
cpg	557.58	J/mol×K	751.42	Joback Method
cpg	571.47	J/mol×K	786.13	Joback Method
hvapt	72.40	kJ/mol	298.15	Vapor pressure and vaporization enthalpy studies of the major components of ginger, alpha-zingiberene, beta-sesquiphellandrene and (-) ar curcumene by correlation gas chromatography

## Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Vapor pressure and vaporization enthalpy studies of the major components of ginger, alpha-zingiberene, beta-sesquiphellandrene and (-) ar curcumene by correlation gas chromatography:

<https://www.doi.org/10.1016/j.jct.2019.06.011>

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C644304&Units=SI>

## Legend

- cpg:** Ideal gas heat capacity  
**gf:** Standard Gibbs free energy of formation  
**hf:** Enthalpy of formation at standard conditions  
**hfus:** Enthalpy of fusion at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>h<sub>vapt</sub>:</b>	Enthalpy of vaporization at a given temperature
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>r<sub>inpol</sub>:</b>	Non-polar retention indices
<b>r<sub>ipol</sub>:</b>	Polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature
<b>t<sub>f</sub>:</b>	Normal melting (fusion) point
<b>v<sub>c</sub>:</b>	Critical Volume

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