

# «gamma»-Curcumenal

<b>Inchi:</b>	InChI=1S/C15H22O/c1-12-7-9-15(10-8-12)14(3)6-4-5-13(2)11-16/h5,7,9,11,14H,4,6,8,10
<b>InchiKey:</b>	ZYTMEMGOUFSSQS-WLRTZDKTSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC(C=O)=CCCC(C)C1=CC=C(C)CC1
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	117.95	kJ/mol	Joback Method
hf	-169.08	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	58.00	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinsol	1742.00		NIST Webbook
tb	627.36	K	Joback Method
tc	836.50	K	Joback Method
tf	304.95	K	Joback Method
vc	0.773	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.46	J/mol×K	627.36	Joback Method
cpg	537.27	J/mol×K	662.22	Joback Method
cpg	554.04	J/mol×K	697.07	Joback Method
cpg	569.80	J/mol×K	731.93	Joback Method
cpg	584.62	J/mol×K	766.79	Joback Method
cpg	598.55	J/mol×K	801.64	Joback Method
cpg	611.63	J/mol×K	836.50	Joback Method

# Sources

<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.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=R287015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R287015&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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