

# Mustakone

**Inchi:** InChI=1S/C15H22O/c1-9-8-10(16)12-13-11(9)15(12,4)7-5-6-14(13,2)3/h8,11-13H,5-7H2,  
**InchiKey:** KTPOZFYJWLGJGH-PYYBWGNESA-N  
**Formula:** C15H22O  
**SMILES:** CC1=CC(=O)C2C3C1C2(C)CCCC3(C)C  
**Mol. weight [g/mol]:** 218.33

## Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	-248.44	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1669.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1670.00		NIST Webbook
tb	634.46	K	Joback Method
tc	873.09	K	Joback Method
tf	426.41	K	Joback Method
vc	0.718	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.90	J/mol×K	634.46	Joback Method
cpg	564.64	J/mol×K	674.23	Joback Method
cpg	585.28	J/mol×K	714.00	Joback Method

cpg	605.11	J/mol×K	753.77	Joback Method
cpg	624.46	J/mol×K	793.54	Joback Method
cpg	643.61	J/mol×K	833.32	Joback Method
cpg	662.89	J/mol×K	873.09	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=R615653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R615653&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>

## 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>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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