

# Elemental

<b>Inchi:</b>	InChI=1S/C15H22O/c1-6-15(5)8-7-13(12(4)10-16)9-14(15)11(2)3/h6,10,13-14H,1-2,4,7-9
<b>InchiKey:</b>	DJZHNAGRSWMVPA-NRXISQOPSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=CC1(C)CCC(C(=C)C=O)CC1C(=C)C</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	225.86	kJ/mol	Joback Method
hf	-52.92	kJ/mol	Joback Method
hfus	18.11	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.926		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
ripol	2084.00		NIST Webbook
ripol	2084.00		NIST Webbook
tb	591.51	K	Joback Method
tc	805.77	K	Joback Method
tf	290.41	K	Joback Method
vc	0.766	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.03	J/mol×K	591.51	Joback Method
cpg	538.42	J/mol×K	627.22	Joback Method
cpg	557.62	J/mol×K	662.93	Joback Method
cpg	575.74	J/mol×K	698.64	Joback Method
cpg	592.90	J/mol×K	734.35	Joback Method
cpg	609.25	J/mol×K	770.06	Joback Method
cpg	624.92	J/mol×K	805.77	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=R327752&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R327752&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>ri pol:</b>	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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