

# (2R,2'S,5R,5'S)-2,5'-Dimethyl-5-(prop-1-en-2-yl)-5'

<b>Inchi:</b>	InChI=1S/C15H22O3/c1-6-14(4)8-7-13(18-14)15(5)12(16)9-11(17-15)10(2)3/h6,11,13H,1
<b>InchiKey:</b>	LQWFUFMRXNEVLA-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O3
<b>SMILES:</b>	C=CC1(C)CCC(C2(C)OC(C=C)C)CC2=O)O1
<b>Mol. weight [g/mol]:</b>	250.33
<b>CAS:</b>	199115-09-8

## Physical Properties

Property code	Value	Unit	Source
gf	-5.58	kJ/mol	Joback Method
hf	-402.80	kJ/mol	Joback Method
hfus	23.62	kJ/mol	Joback Method
hvap	58.59	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.803		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1532.60		NIST Webbook
rinpol	1532.60		NIST Webbook
tb	679.26	K	Joback Method
tc	921.44	K	Joback Method
tf	423.81	K	Joback Method
vc	0.763	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.67	J/molxK	679.26	Joback Method
cpg	628.38	J/molxK	719.62	Joback Method
cpg	649.17	J/molxK	759.99	Joback Method
cpg	669.31	J/molxK	800.35	Joback Method
cpg	689.07	J/molxK	840.72	Joback Method
cpg	708.72	J/molxK	881.08	Joback Method
cpg	728.55	J/molxK	921.44	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C199115098&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C199115098&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>

# 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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