

# (+)-(4S,5S,6S,7S)-Plagiochiline W

<b>Inchi:</b>	InChI=1S/C15H22O/c1-9-5-6-12-14(15(12,3)4)13-10(2)7-16-8-11(9)13/h5,8,10,12-14H,6
<b>InchiKey:</b>	PEDRFNLMEGPQLB-SAXRGWBVSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC1=CCC2C(C3C1=COCC3C)C2(C)C
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	155.00	kJ/mol	Joback Method
hf	-217.83	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Joback Method
hvap	53.89	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.775		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
tb	601.76	K	Joback Method
tc	826.79	K	Joback Method
tf	370.62	K	Joback Method
vc	0.712	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.34	J/mol×K	601.76	Joback Method
cpg	543.89	J/mol×K	639.27	Joback Method
cpg	564.09	J/mol×K	676.77	Joback Method
cpg	583.14	J/mol×K	714.28	Joback Method
cpg	601.22	J/mol×K	751.78	Joback Method
cpg	618.50	J/mol×K	789.29	Joback Method
cpg	635.16	J/mol×K	826.79	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=R561363&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R561363&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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