

# (+)-(5S,6S,7S)-Plagiochiline X

<b>Inchi:</b>	InChI=1S/C15H20O/c1-9-5-6-12-14(15(12,3)4)13-10(2)7-16-8-11(9)13/h5,8,12-14H,2,6-7
<b>InchiKey:</b>	MPCQKDYHFFZZAW-IHRRRGAJSA-N
<b>Formula:</b>	C15H20O
<b>SMILES:</b>	C=C1COC=C2C(C)=CCC3C(C12)C3(C)C
<b>Mol. weight [g/mol]:</b>	216.32

## Physical Properties

Property code	Value	Unit	Source
gf	215.79	kJ/mol	Joback Method
hf	-113.25	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	54.36	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.695		Crippen Method
mvol	182.600	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	605.59	K	Joback Method
tc	832.53	K	Joback Method
tf	388.54	K	Joback Method
vc	0.697	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.21	J/molxK	605.59	Joback Method
cpg	519.05	J/molxK	643.41	Joback Method
cpg	537.65	J/molxK	681.24	Joback Method
cpg	555.20	J/molxK	719.06	Joback Method
cpg	571.88	J/molxK	756.89	Joback Method
cpg	587.87	J/molxK	794.71	Joback Method
cpg	603.36	J/molxK	832.53	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=R561407&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R561407&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>
<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>r in pol:</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

Latest version available from:

<https://www.cheméo.com/cid/31-155-5/5S-6S-7S-Plagiochiline-X.pdf>

Generated by Cheméo on 2024-05-04 02:07:23.746536131 +0000 UTC m=+17077692.667113442.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.