

(+)-Plagiochiline W

Inchi:	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
InchiKey:	PEDRFNLMEGPQLB-AHLYJBGZSA-N
Formula:	C15H22O
SMILES:	CC1=CCC2C(C3C1=COCC3C)C2(C)C
Mol. weight [g/mol]:	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
rmpol	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 ³ /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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R411357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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