

# Cyperadiene

<b>Inchi:</b>	InChI=1S/C15H22/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h7-8,11-13H,1,5-6,9H
<b>InchiKey:</b>	KZABVHBACHSSNR-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	<chem>C=C1C=CC23C(C)CCC(CC12)C3(C)C</chem>
<b>Mol. weight [g/mol]:</b>	202.34
<b>CAS:</b>	394217-21-1

## Physical Properties

Property code	Value	Unit	Source
gf	290.11	kJ/mol	Joback Method
hf	-15.03	kJ/mol	Joback Method
hfus	14.42	kJ/mol	Joback Method
hvap	46.60	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.191		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1442.70		NIST Webbook
tb	560.82	K	Joback Method
tc	787.28	K	Joback Method
tf	359.35	K	Joback Method
vc	0.695	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.51	J/molxK	560.82	Joback Method
cpg	504.64	J/molxK	598.56	Joback Method
cpg	525.18	J/molxK	636.31	Joback Method
cpg	544.42	J/molxK	674.05	Joback Method
cpg	562.67	J/molxK	711.80	Joback Method
cpg	580.23	J/molxK	749.54	Joback Method

## Sources

<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=C394217211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C394217211&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>

## 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>hvap:</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>rinpol:</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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