

# Isocembrene

<b>Inchi:</b>	InChI=1S/C20H32/c1-16(2)20-14-12-18(4)10-6-8-17(3)9-7-11-19(5)13-15-20/h8,11-12,14
<b>InchiKey:</b>	VYWGLUCGRVXWKB-KSJQBYEHS-A-N
<b>Formula:</b>	C20H32
<b>SMILES:</b>	<chem>C=C1C=CC(C(C)C)CCC(C)=CCCC(C)=CCC1</chem>
<b>Mol. weight [g/mol]:</b>	272.47

## Physical Properties

Property code	Value	Unit	Source
gf	166.43	kJ/mol	Joback Method
hf	-221.73	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	6.618		Crippen Method
mcvol	264.600	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1945.00		NIST Webbook
ripol	2297.00		NIST Webbook
ripol	2297.00		NIST Webbook
tb	716.87	K	Joback Method
tc	950.69	K	Joback Method
tf	320.38	K	Joback Method
vc	0.961	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.20	J/molxK	716.87	Joback Method
cpg	885.57	J/molxK	911.72	Joback Method
cpg	867.27	J/molxK	872.75	Joback Method
cpg	846.85	J/molxK	833.78	Joback Method

cpg	824.35	J/molxK	794.81	Joback Method
cpg	799.79	J/molxK	755.84	Joback Method
cpg	901.74	J/molxK	950.69	Joback Method
dvisc	0.0000099	Paxs	716.87	Joback Method
dvisc	0.0000163	Paxs	650.79	Joback Method
dvisc	0.0000301	Paxs	584.71	Joback Method
dvisc	0.0000649	Paxs	518.62	Joback Method
dvisc	0.0001748	Paxs	452.54	Joback Method
dvisc	0.0006609	Paxs	386.46	Joback Method
dvisc	0.0043264	Paxs	320.38	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=R429704&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R429704&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>ripol:</b>	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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