

# Brazila-1(6),5(1)-diene

<b>Inchi:</b>	InChI=1S/C15H24/c1-10(2)13-8-15(4,5)9-14-11(3)6-7-12(13)14/h11H,6-9H2,1-5H3/t11-/r
<b>InchiKey:</b>	XLVUTANZHOECMR-NSHDSACASA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC(C)=C1CC(C)(C)CC2=C1CCC2C
<b>Mol. weight [g/mol]:</b>	204.35

## Physical Properties

Property code	Value	Unit	Source
gf	202.74	kJ/mol	Joback Method
hf	-109.49	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	50.66	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinsol	1436.00		NIST Webbook
tb	584.77	K	Joback Method
tc	805.24	K	Joback Method
tf	330.23	K	Joback Method
vc	0.734	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.81	J/mol×K	584.77	Joback Method
cpg	520.83	J/mol×K	621.52	Joback Method
cpg	540.61	J/mol×K	658.26	Joback Method
cpg	559.31	J/mol×K	695.01	Joback Method
cpg	577.08	J/mol×K	731.75	Joback Method
cpg	594.09	J/mol×K	768.50	Joback Method
cpg	610.49	J/mol×K	805.24	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=R589014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R589014&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>
<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>rinpola:</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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