

# African-2,6-diene

<b>Inchi:</b>	InChI=1S/C15H22/c1-10-5-6-13-12(10)9-14(2,3)7-11-8-15(11,13)4/h6,9-11H,5,7-8H2,1-4
<b>InchiKey:</b>	RPHSOXQGRPSCDV-VIBFFUDUSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	CC1CC=C2C1=CC(C)(C)CC1CC21C
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	255.44	kJ/mol	Joback Method
hf	-44.09	kJ/mol	Joback Method
hfus	14.95	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	575.45	K	Joback Method
tc	804.27	K	Joback Method
tf	375.71	K	Joback Method
vc	0.698	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.52	J/mol×K	575.45	Joback Method
cpg	504.45	J/mol×K	613.59	Joback Method
cpg	523.95	J/mol×K	651.72	Joback Method
cpg	542.31	J/mol×K	689.86	Joback Method
cpg	559.86	J/mol×K	728.00	Joback Method
cpg	576.90	J/mol×K	766.14	Joback Method
cpg	593.73	J/mol×K	804.27	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=R588982&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R588982&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.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

Latest version available from:

<https://www.chemeo.com/cid/28-392-6/African-2-6-diene.pdf>

Generated by Cheméo on 2024-04-28 21:44:10.528320445 +0000 UTC m=+16629899.448897772.

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