

# Oppositadiene

**Inchi:** InChI=1S/C15H24/c1-11(2)10-13-7-9-15(4)8-5-6-12(3)14(13)15/h10,13-14H,3,5-9H2,1-2  
**InchiKey:** VDZLIVJTPHFVKL-KKUMJFAQSA-N  
**Formula:** C15H24  
**SMILES:** C=C1CCCC2(C)CCC(C=C(C)C)C12  
**Mol. weight [g/mol]:** 204.35

## Physical Properties

Property code	Value	Unit	Source
gf	272.17	kJ/mol	Joback Method
hf	-39.24	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1393.00		NIST Webbook
tb	567.66	K	Joback Method
tc	788.60	K	Joback Method
tf	298.43	K	Joback Method
vc	0.728	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.58	J/molxK	567.66	Joback Method
cpg	521.39	J/molxK	604.48	Joback Method
cpg	542.75	J/molxK	641.31	Joback Method
cpg	562.82	J/molxK	678.13	Joback Method
cpg	581.77	J/molxK	714.95	Joback Method
cpg	599.77	J/molxK	751.77	Joback Method
cpg	616.99	J/molxK	788.60	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R571558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R571558&amp;Units=SI</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>hvp:</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>rinp:</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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