

# trans-caryophyllene oxide

<b>Other names:</b>	trans-Caryophyllene epoxide trans- «beta»-Caryophyllene oxide
<b>Inchi:</b>	InChI=1S/C15H24O/c1-10-5-6-13-15(4,16-13)8-7-12-11(10)9-14(12,2)3/h11-13H,1,5-9H
<b>InchiKey:</b>	NVEQFIOZRFFVFW-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC2OC2(C)CCC2C1CC2(C)C</chem>
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	161.93	kJ/mol	Joback Method
hf	-210.97	kJ/mol	Joback Method
hfus	19.08	kJ/mol	Joback Method
hvap	50.99	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.936		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1583.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook
ripol	1962.00		NIST Webbook
tb	592.88	K	Joback Method
tc	822.50	K	Joback Method
tf	381.64	K	Joback Method
vc	0.722	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.37	J/mol×K	592.88	Joback Method
cpg	562.46	J/mol×K	631.15	Joback Method
cpg	584.07	J/mol×K	669.42	Joback Method
cpg	604.52	J/mol×K	707.69	Joback Method
cpg	624.09	J/mol×K	745.96	Joback Method
cpg	643.08	J/mol×K	784.23	Joback Method
cpg	661.78	J/mol×K	822.50	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R235811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R235811&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>
<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>

## 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>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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