

# epoxy citronellene

<b>Inchi:</b>	InChI=1S/C10H18O/c1-5-8(2)6-7-9-10(3,4)11-9/h5,8-9H,1,6-7H2,2-4H3
<b>InchiKey:</b>	IQTYEDULQISSGT-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O
<b>SMILES:</b>	C=CC(C)CCC1OC1(C)C
<b>Mol. weight [g/mol]:</b>	154.25

## Physical Properties

Property code	Value	Unit	Source
gf	80.15	kJ/mol	Joback Method
hf	-193.88	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	39.76	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.766		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	453.70	K	Joback Method
tc	644.30	K	Joback Method
tf	249.87	K	Joback Method
vc	0.545	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.19	J/mol×K	453.70	Joback Method
cpg	334.68	J/mol×K	485.47	Joback Method
cpg	350.12	J/mol×K	517.23	Joback Method
cpg	364.59	J/mol×K	549.00	Joback Method
cpg	378.19	J/mol×K	580.76	Joback Method
cpg	391.01	J/mol×K	612.53	Joback Method
cpg	403.16	J/mol×K	644.30	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=R199463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R199463&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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