

# (+)-6,11-Epoxy-eudesmane

<b>Inchi:</b>	InChI=1S/C16H28O/c1-11-6-5-8-16(4)9-7-13-12(14(11)16)10-17-15(13,2)3/h11-14H,5-10
<b>InchiKey:</b>	NTLMTFAQVVZEQY-UHFFFAOYSA-N
<b>Formula:</b>	C16H28O
<b>SMILES:</b>	CC1CCCC2(C)CCC3C(COC3(C)C)C12
<b>Mol. weight [g/mol]:</b>	236.39

## Physical Properties

Property code	Value	Unit	Source
gf	97.46	kJ/mol	Joback Method
hf	-342.35	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.264		Crippen Method
mvol	209.590	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	616.20	K	Joback Method
tc	847.19	K	Joback Method
tf	371.47	K	Joback Method
vc	0.784	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.87	J/mol×K	616.20	Joback Method
cpg	644.95	J/mol×K	654.70	Joback Method
cpg	669.49	J/mol×K	693.20	Joback Method
cpg	692.80	J/mol×K	731.70	Joback Method
cpg	715.16	J/mol×K	770.19	Joback Method
cpg	736.87	J/mol×K	808.69	Joback Method
cpg	758.22	J/mol×K	847.19	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=R504320&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R504320&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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