

# 6,12;7,11-Diepoxy-eudesm-4-ene (epimer B)

Inchi:	InChI=1S/C15H22O2/c1-10-5-4-6-13(2)7-8-15-12(11(10)13)16-9-14(15,3)17-15/h12H,4-9
InchiKey:	JFQRIENZNRVMS-MXTXEEQBSA-N
Formula:	C15H22O2
SMILES:	CC1=C2C3OCC4(C)OC34CCC2(C)CCC1
Mol. weight [g/mol]:	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	116.21	kJ/mol	Joback Method
hf	-257.49	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	56.16	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.213		Crippen Method
mcvol	186.210	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1753.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2410.00		NIST Webbook
tb	641.84	K	Joback Method
tc	888.44	K	Joback Method
tf	474.17	K	Joback Method
vc	0.710	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.07	J/molxK	641.84	Joback Method
cpg	573.12	J/molxK	682.94	Joback Method
cpg	592.26	J/molxK	724.04	Joback Method
cpg	611.07	J/molxK	765.14	Joback Method
cpg	630.08	J/molxK	806.24	Joback Method

cpg	649.87	J/mol×K	847.34	Joback Method
cpg	670.97	J/mol×K	888.44	Joback Method

## Sources

<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=R236092&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R236092&amp;Units=SI</a>
<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.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>

## 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>ripola:</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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