

# (+)-(7S,8R,9S,10R)-8,9-Epoxyseleina-4,11-diene

<b>Inchi:</b>	InChI=1S/C15H22O/c1-9(2)11-8-12-10(3)6-5-7-15(12,4)14-13(11)16-14/h11,13-14H,1,5-
<b>InchiKey:</b>	HPCVVOEQSOLQFPZ-MXAVVETBSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	<chem>C=C(C)C1CC2=C(C)CCCC2(C)C2OC12</chem>
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	224.14	kJ/mol	Joback Method
hf	-133.47	kJ/mol	Joback Method
hfus	25.42	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinsol	1596.00		NIST Webbook
tb	599.56	K	Joback Method
tc	823.57	K	Joback Method
tf	361.90	K	Joback Method
vc	0.717	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.44	J/molxK	599.56	Joback Method
cpg	539.34	J/molxK	636.89	Joback Method
cpg	558.90	J/molxK	674.23	Joback Method
cpg	577.33	J/molxK	711.56	Joback Method
cpg	594.83	J/molxK	748.90	Joback Method
cpg	611.59	J/molxK	786.23	Joback Method
cpg	627.81	J/molxK	823.57	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R561447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R561447&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvac:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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