

# (-)-7-epi-Eremophila-1(10),8,11-triene

<b>Inchi:</b>	InChI=1S/C15H22/c1-11(2)13-8-9-14-7-5-6-12(3)15(14,4)10-13/h7-9,12-13H,1,5-6,10H2
<b>InchiKey:</b>	DQPQHEZYSQLQOQ-KCQAQPDRSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	C=C(C)C1C=CC2=CCCC(C)C2(C)C1
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	264.90	kJ/mol	Joback Method
hf	-17.34	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	48.69	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.501		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1507.00		NIST Webbook
tb	568.59	K	Joback Method
tc	795.68	K	Joback Method
tf	298.59	K	Joback Method
vc	0.709	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.93	J/molxK	568.59	Joback Method
cpg	502.32	J/molxK	606.44	Joback Method
cpg	523.23	J/molxK	644.29	Joback Method
cpg	542.85	J/molxK	682.13	Joback Method
cpg	561.34	J/molxK	719.98	Joback Method
cpg	578.86	J/molxK	757.83	Joback Method
cpg	595.59	J/molxK	795.68	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=R283895&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R283895&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.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>

# 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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