

# 2,5-Etheno[4.2.2]propella-3,7,9-triene

<b>Inchi:</b>	InChI=1S/C12H10/c1-2-10-4-3-9(1)11-5-7-12(10,11)8-6-11/h1-10H
<b>InchiKey:</b>	RDIUVVQMLJOTAO-UHFFFAOYSA-N
<b>Formula:</b>	C12H10
<b>SMILES:</b>	C1=CC2C=CC1C13C=CC21C=C3
<b>Mol. weight [g/mol]:</b>	154.21
<b>CAS:</b>	88090-38-4

## Physical Properties

Property code	Value	Unit	Source
gf	402.02	kJ/mol	Joback Method
hf	261.79	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	40.82	kJ/mol	Joback Method
ie	8.14	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.87		Crippen Method
logp	2.471		Crippen Method
mcvol	119.300	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	498.04	K	Joback Method
tc	744.15	K	Joback Method
tf	347.60	K	Joback Method
vc	0.475	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.56	J/molxK	498.04	Joback Method
cpg	303.41	J/molxK	539.06	Joback Method
cpg	317.98	J/molxK	580.08	Joback Method
cpg	330.74	J/molxK	621.10	Joback Method
cpg	342.16	J/molxK	662.11	Joback Method
cpg	352.73	J/molxK	703.13	Joback Method
cpg	362.90	J/molxK	744.15	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.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=C88090384&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C88090384&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>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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>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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