

# Oxirane,trans-2,3-diethynyl-

<b>Inchi:</b>	InChI=1S/C5H3NO/c1-2-4-5(3-6)7-4/h1,4-5H/t4-,5-/m0/s1
<b>InchiKey:</b>	TTYKBHXCNCFTQB-WHFBIAKZSA-N
<b>Formula:</b>	C6H4O
<b>SMILES:</b>	C#CC1OC1C#N
<b>Mol. weight [g/mol]:</b>	92.10
<b>CAS:</b>	40020-14-2

## Physical Properties

Property code	Value	Unit	Source
gf	314.39	kJ/mol	Joback Method
hf	230.71	kJ/mol	Joback Method
hfus	20.37	kJ/mol	Joback Method
hvap	41.17	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
log10ws	-0.78		Crippen Method
logp	-0.089		Crippen Method
mcvol	69.100	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	435.02	K	Joback Method
tc	657.56	K	Joback Method
tf	298.34	K	Joback Method
vc	0.281	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.25	J/molxK	435.02	Joback Method
cpg	142.17	J/molxK	472.11	Joback Method
cpg	148.57	J/molxK	509.20	Joback Method
cpg	154.49	J/molxK	546.29	Joback Method
cpg	159.96	J/molxK	583.38	Joback Method
cpg	165.01	J/molxK	620.47	Joback Method
cpg	169.70	J/molxK	657.56	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=C40020142&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40020142&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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