

# But-1-ene-3-yne, 1-ethoxy-

<b>Inchi:</b>	InChI=1S/C6H8O/c1-3-5-6-7-4-2/h1,5-6H,4H2,2H3/b6-5+
<b>InchiKey:</b>	LYWWXPVUSWJFCZ-AATRIKPKSA-N
<b>Formula:</b>	C6H8O
<b>SMILES:</b>	C#CC=COCC
<b>Mol. weight [g/mol]:</b>	96.13
<b>CAS:</b>	2806-41-9

## Physical Properties

Property code	Value	Unit	Source
gf	197.93	kJ/mol	Joback Method
hf	109.73	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	31.18	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.170		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
tb	353.38	K	Joback Method
tc	539.48	K	Joback Method
tf	221.50	K	Joback Method
vc	0.332	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.12	J/molxK	353.38	Joback Method
cpg	154.36	J/molxK	384.40	Joback Method
cpg	162.23	J/molxK	415.41	Joback Method
cpg	169.75	J/molxK	446.43	Joback Method
cpg	176.94	J/molxK	477.44	Joback Method
cpg	183.80	J/molxK	508.46	Joback Method
cpg	190.34	J/molxK	539.48	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=C2806419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2806419&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>

# 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>mccol:</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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