

# CH2CCH

<b>Inchi:</b>	InChI=1S/C3H3/c1-3-2/h1H,2H2
<b>InchiKey:</b>	DITHIFQMPPCBCU-UHFFFAOYSA-N
<b>Formula:</b>	C3H3
<b>SMILES:</b>	[CH]=C=C
<b>Mol. weight [g/mol]:</b>	39.06
<b>CAS:</b>	6401-87-2

## Physical Properties

Property code	Value	Unit	Source
gf	242.88	kJ/mol	Joback Method
hf	238.77	kJ/mol	Joback Method
hfus	6.06	kJ/mol	Joback Method
hvap	21.89	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.760		Crippen Method
mcvol	42.380	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	267.29	K	Joback Method
tc	438.80	K	Joback Method
tf	144.69	K	Joback Method
vc	0.155	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	50.57	J/molxK	267.29	Joback Method
cpg	54.05	J/molxK	295.87	Joback Method
cpg	57.30	J/molxK	324.46	Joback Method
cpg	60.34	J/molxK	353.04	Joback Method
cpg	63.19	J/molxK	381.63	Joback Method
cpg	65.85	J/molxK	410.21	Joback Method
cpg	68.34	J/molxK	438.80	Joback Method

# Sources

<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.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=C6401872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6401872&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>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>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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