

# Cyclobutanecarboxylic acid, pent-2-en-4-ynyl ester

Inchi:	InChI=1S/C10H12O2/c1-2-3-4-8-12-10(11)9-6-5-7-9/h1,3-4,9H,5-8H2
InchiKey:	DVNOPGBSYJNWPM-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	C#CC=CCOC(=O)C1CCC1
Mol. weight [g/mol]:	164.20

## Physical Properties

Property code	Value	Unit	Source
gf	151.34	kJ/mol	Joback Method
hf	-18.77	kJ/mol	Joback Method
hfus	23.65	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.519		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinsol	1244.00		NIST Webbook
tb	509.78	K	Joback Method
tc	724.28	K	Joback Method
tf	330.93	K	Joback Method
vc	0.510	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.35	J/mol×K	509.78	Joback Method
cpg	315.65	J/mol×K	545.53	Joback Method
cpg	329.06	J/mol×K	581.28	Joback Method
cpg	341.62	J/mol×K	617.03	Joback Method
cpg	353.37	J/mol×K	652.78	Joback Method
cpg	364.38	J/mol×K	688.53	Joback Method
cpg	374.69	J/mol×K	724.28	Joback Method

# Sources

<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=U299130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299130&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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