

# C11H18O2

<b>Inchi:</b>	InChI=1S/C11H18O2/c1-3-5-6-7-8-9-10-11(12)13-4-2/h3-8H2,1-2H3
<b>InchiKey:</b>	BFZNMUGAZYAMTG-UHFFFAOYSA-N
<b>Formula:</b>	C11H18O2
<b>SMILES:</b>	CCCCCCC#CC(=O)OCC
<b>Mol. weight [g/mol]:</b>	182.26
<b>CAS:</b>	1322-12-9

## Physical Properties

Property code	Value	Unit	Source
gf	10.62	kJ/mol	Joback Method
hf	-242.87	kJ/mol	Joback Method
hfus	30.16	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.523		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	536.37	K	Joback Method
tc	727.55	K	Joback Method
tf	391.99	K	Joback Method
vc	0.637	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.50	J/molxK	536.37	Joback Method
cpg	394.84	J/molxK	568.23	Joback Method
cpg	408.58	J/molxK	600.10	Joback Method
cpg	421.74	J/molxK	631.96	Joback Method
cpg	434.31	J/molxK	663.82	Joback Method
cpg	446.31	J/molxK	695.69	Joback Method
cpg	457.74	J/molxK	727.55	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=C1322129&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1322129&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>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>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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