

# (E),(Z)-pseudoionone

<b>Inchi:</b>	InChI=1S/C13H22O/c1-11(2)7-5-8-12(3)9-6-10-13(4)14/h6,9-11H,5,7-8H2,1-4H3
<b>InchiKey:</b>	HBZBROBMQHQJIBO-UHFFFAOYSA-N
<b>Formula:</b>	C13H22O
<b>SMILES:</b>	CC(=O)C=CC=C(C)CCCC(C)C
<b>Mol. weight [g/mol]:</b>	194.31

## Physical Properties

Property code	Value	Unit	Source
gf	79.11	kJ/mol	Joback Method
hf	-204.86	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.904		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
ripol	1995.00		NIST Webbook
ripol	1995.00		NIST Webbook
tb	558.47	K	Joback Method
tc	747.82	K	Joback Method
tf	247.08	K	Joback Method
vc	0.725	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.37	J/molxK	558.47	Joback Method
cpg	465.86	J/molxK	590.03	Joback Method
cpg	481.50	J/molxK	621.59	Joback Method
cpg	496.33	J/molxK	653.15	Joback Method
cpg	510.38	J/molxK	684.71	Joback Method
cpg	523.71	J/molxK	716.27	Joback Method
cpg	536.36	J/molxK	747.82	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=R494852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R494852&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>ri pol:</b>	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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