

# Tetrahydroionone

<b>Inchi:</b>	InChI=1S/C13H24O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h10,12H,5-9H2,1-4H3
<b>InchiKey:</b>	PQCDGQHNORPNBR-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O
<b>SMILES:</b>	CC(=O)CCC1C(C)CCCC1(C)C
<b>Mol. weight [g/mol]:</b>	196.33
<b>CAS:</b>	60761-23-1

## Physical Properties

Property code	Value	Unit	Source
gf	-66.80	kJ/mol	Joback Method
hf	-395.35	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.818		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1427.10		NIST Webbook
rinpol	1427.10		NIST Webbook
tb	561.16	K	Joback Method
tc	766.91	K	Joback Method
tf	309.00	K	Joback Method
vc	0.699	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.29	J/molxK	561.16	Joback Method
cpg	498.16	J/molxK	595.45	Joback Method
cpg	517.90	J/molxK	629.74	Joback Method
cpg	536.62	J/molxK	664.03	Joback Method
cpg	554.39	J/molxK	698.33	Joback Method
cpg	571.32	J/molxK	732.62	Joback Method
cpg	587.49	J/molxK	766.91	Joback Method

# Sources

<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=C60761231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60761231&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>r in pol:</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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