

# 3-oxo-«alpha»-retroionol 1

<b>Inchi:</b>	InChI=1S/C13H20O2/c1-9-7-11(15)8-13(3,4)12(9)6-5-10(2)14/h6-7,10,14H,5,8H2,1-4H3
<b>InchiKey:</b>	JHWWVZZGBLPJPW-SDQBPNPISA-N
<b>Formula:</b>	C13H20O2
<b>SMILES:</b>	CC1=CC(=O)CC(C)(C)C1=CCC(C)O
<b>Mol. weight [g/mol]:</b>	208.30

## Physical Properties

Property code	Value	Unit	Source
gf	-118.52	kJ/mol	Joback Method
hf	-414.96	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	66.09	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
ripol	2756.00		NIST Webbook
tb	686.97	K	Joback Method
tc	896.30	K	Joback Method
tf	405.23	K	Joback Method
vc	0.683	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.30	J/molxK	686.97	Joback Method
cpg	524.83	J/molxK	721.86	Joback Method
cpg	539.71	J/molxK	756.75	Joback Method
cpg	554.03	J/molxK	791.64	Joback Method
cpg	567.87	J/molxK	826.52	Joback Method
cpg	581.31	J/molxK	861.41	Joback Method
cpg	594.44	J/molxK	896.30	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=R332957&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R332957&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</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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