

# 4-oxo-«beta»-ionol

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

## Physical Properties

Property code	Value	Unit	Source
gf	-93.39	kJ/mol	Joback Method
hf	-385.24	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	65.92	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.629		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
ripol	1660.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1660.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2630.00		NIST Webbook
tb	689.47	K	Joback Method
tc	901.80	K	Joback Method
tf	402.31	K	Joback Method
vc	0.680	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.79	J/mol×K	689.47	Joback Method
cpg	525.56	J/mol×K	724.86	Joback Method
cpg	540.68	J/mol×K	760.25	Joback Method
cpg	555.22	J/mol×K	795.64	Joback Method
cpg	569.29	J/mol×K	831.02	Joback Method
cpg	582.97	J/mol×K	866.41	Joback Method
cpg	596.37	J/mol×K	901.80	Joback Method

## Sources

<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>
<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=R272870&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R272870&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>	Non-polar retention indices
<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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