

# ( Z)-vertocitral C

<b>Other names:</b>	(E)-vertocitral C
<b>Inchi:</b>	InChI=1S/C9H14O/c1-7-3-4-9(6-10)8(2)5-7/h5-6,8-9H,3-4H2,1-2H3/t8?,9-/m0/s1
<b>InchiKey:</b>	MZZRKEIUNOYYDF-GKAPJAKFSA-N
<b>Formula:</b>	C9H14O
<b>SMILES:</b>	<chem>CC1=CC(C)C(C=O)CC1</chem>
<b>Mol. weight [g/mol]:</b>	138.21
<b>CAS:</b>	65405-78-9

## Physical Properties

Property code	Value	Unit	Source
gf	-37.55	kJ/mol	Joback Method
hf	-234.38	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
tb	473.00	K	Joback Method
tc	680.91	K	Joback Method
tf	249.61	K	Joback Method
vc	0.474	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.51	J/molxK	473.00	Joback Method
cpg	284.31	J/molxK	507.65	Joback Method
cpg	299.34	J/molxK	542.30	Joback Method
cpg	313.61	J/molxK	576.96	Joback Method
cpg	327.13	J/molxK	611.61	Joback Method
cpg	339.93	J/molxK	646.26	Joback Method

cpg	352.00	J/mol×K	680.91	Joback Method
dvisc	0.0025258	Paxs	249.61	Joback Method
dvisc	0.0014404	Paxs	286.84	Joback Method
dvisc	0.0009346	Paxs	324.07	Joback Method
dvisc	0.0006629	Paxs	361.31	Joback Method
dvisc	0.0005014	Paxs	398.54	Joback Method
dvisc	0.0003978	Paxs	435.77	Joback Method
dvisc	0.0003273	Paxs	473.00	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=C65405789&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C65405789&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>
<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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>rinpol:</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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