

# 6-hydroxycarvotanacetone

<b>Inchi:</b>	InChI=1S/C10H16O2/c1-6(2)8-5-4-7(3)9(11)10(8)12/h4,6,8,10,12H,5H2,1-3H3
<b>InchiKey:</b>	CSTXLFNLXWTVDQ-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O2
<b>SMILES:</b>	CC1=CCC(C(C)C)C(O)C1=O
<b>Mol. weight [g/mol]:</b>	168.23
<b>CAS:</b>	131486-99-2

## Physical Properties

Property code	Value	Unit	Source
gf	-191.46	kJ/mol	Joback Method
hf	-464.65	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	59.47	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.539		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1317.80		NIST Webbook
rinpol	1317.80		NIST Webbook
tb	606.78	K	Joback Method
tc	812.40	K	Joback Method
tf	332.92	K	Joback Method
vc	0.533	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.06	J/mol×K	606.78	Joback Method
cpg	398.33	J/mol×K	641.05	Joback Method
cpg	412.83	J/mol×K	675.32	Joback Method
cpg	426.57	J/mol×K	709.59	Joback Method
cpg	439.53	J/mol×K	743.86	Joback Method
cpg	451.71	J/mol×K	778.13	Joback Method
cpg	463.09	J/mol×K	812.40	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=C131486992&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C131486992&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.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>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>rinpola:</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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