

# trans-Chrysanthamal

<b>Inchi:</b>	InChI=1S/C10H16O/c1-7(2)5-8-9(6-11)10(8,3)4/h5-6,8-9H,1-4H3/t8-,9-/m0/s1
<b>InchiKey:</b>	NQLKPDBZZUIQGM-IUCAKERBSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	CC(C)=CC1C(C=O)C1(C)C
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	20104-05-6

## Physical Properties

Property code	Value	Unit	Source
gf	45.31	kJ/mol	Joback Method
hf	-180.52	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	42.76	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1153.00		NIST Webbook
tb	478.54	K	Joback Method
tc	679.18	K	Joback Method
tf	258.78	K	Joback Method
vc	0.546	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.37	J/molxK	478.54	Joback Method
cpg	329.20	J/molxK	511.98	Joback Method
cpg	343.97	J/molxK	545.42	Joback Method
cpg	357.77	J/molxK	578.86	Joback Method
cpg	370.71	J/molxK	612.30	Joback Method

cpg	382.92	J/mol×K	645.74	Joback Method
cpg	394.51	J/mol×K	679.18	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=C20104056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20104056&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>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>rinpolar:</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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