

# Dolichodial

**Inchi:** InChI=1S/C10H14O2/c1-7-3-4-9(8(2)5-11)10(7)6-12/h5-7,9-10H,2-4H2,1H3/t7-,9?,10?/m  
**InchiKey:** BORBLDJNKYHVJP-WFRXLMHJSA-N  
**Formula:** C10H14O2  
**SMILES:** C=C(C=O)C1CCC(C)C1C=O  
**Mol. weight [g/mol]:** 166.22

## Physical Properties

Property code	Value	Unit	Source
gf	-65.30	kJ/mol	Joback Method
hf	-285.45	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	50.34	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.603		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
tb	528.02	K	Joback Method
tc	734.55	K	Joback Method
tf	273.16	K	Joback Method
vc	0.550	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.76	J/mol×K	528.02	Joback Method
cpg	351.54	J/mol×K	562.44	Joback Method
cpg	366.44	J/mol×K	596.86	Joback Method
cpg	380.49	J/mol×K	631.28	Joback Method
cpg	393.72	J/mol×K	665.70	Joback Method
cpg	406.15	J/mol×K	700.13	Joback Method
cpg	417.81	J/mol×K	734.55	Joback Method

# Sources

<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=R345176&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R345176&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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