

# iso-Amyl tiglate

<b>Inchi:</b>	InChI=1S/C10H18O2/c1-5-9(4)10(11)12-7-6-8(2)3/h5,8H,6-7H2,1-4H3/b9-5-
<b>InchiKey:</b>	ZARFDQHJMNVNLE-UITAMQMPSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	CC=C(C)C(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	170.25
<b>CAS:</b>	66917-62-2

## Physical Properties

Property code	Value	Unit	Source
gf	-131.37	kJ/mol	Joback Method
hf	-392.38	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1178.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1471.00		NIST Webbook
tb	508.09	K	Joback Method
tc	694.82	K	Joback Method
tf	240.58	K	Joback Method
vc	0.595	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.82	J/molxK	508.09	Joback Method
cpg	365.21	J/molxK	539.21	Joback Method
cpg	378.95	J/molxK	570.33	Joback Method
cpg	392.08	J/molxK	601.46	Joback Method
cpg	404.60	J/molxK	632.58	Joback Method
cpg	416.53	J/molxK	663.70	Joback Method

## Sources

<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=C66917622&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C66917622&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>

## 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>rinpol:</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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