

# trans-5-Methyl-2-isopropyl-2-hexen-1-al

<b>Other names:</b>	E-2-Hexenal, 5-methyl-2-(1-methylethyl)-
<b>Inchi:</b>	InChI=1S/C10H18O/c1-8(2)5-6-10(7-11)9(3)4/h6-9H,5H2,1-4H3/b10-6-
<b>InchiKey:</b>	IOLQAHFPDADCHJ-POHAHGRESA-N
<b>Formula:</b>	C10H18O
<b>SMILES:</b>	CC(C)CC=C(C=O)C(C)C
<b>Mol. weight [g/mol]:</b>	154.25

## Physical Properties

Property code	Value	Unit	Source
gf	0.59	kJ/mol	Joback Method
hf	-238.44	kJ/mol	Joback Method
hfus	15.79	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.814		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	480.02	K	Joback Method
tc	667.13	K	Joback Method
tf	195.42	K	Joback Method
vc	0.582	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.28	J/molxK	480.02	Joback Method
cpg	341.03	J/molxK	511.21	Joback Method
cpg	355.07	J/molxK	542.39	Joback Method
cpg	368.41	J/molxK	573.58	Joback Method
cpg	381.09	J/molxK	604.76	Joback Method
cpg	393.14	J/molxK	635.95	Joback Method
cpg	404.58	J/molxK	667.13	Joback Method

# Sources

<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>
<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=U139661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U139661&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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