

# 3,5-Heptadienol, 2-ethylidene-6-methyl, isomer # 1

Inchi:	InChI=1S/C10H16O/c1-4-10(8-11)7-5-6-9(2)3/h4-7,11H,8H2,1-3H3
InchiKey:	FSTMFKMUZPMDAZ-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC=C(C=CC=C(C)C)CO
Mol. weight [g/mol]:	152.23

## Physical Properties

Property code	Value	Unit	Source
gf	120.06	kJ/mol	Joback Method
hf	-69.88	kJ/mol	Joback Method
hfus	23.73	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.447		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1195.00		NIST Webbook
tb	532.62	K	Joback Method
tc	717.13	K	Joback Method
tf	220.12	K	Joback Method
vc	0.556	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.14	J/mol×K	532.62	Joback Method
cpg	338.48	J/mol×K	563.37	Joback Method
cpg	350.12	J/mol×K	594.12	Joback Method
cpg	361.13	J/mol×K	624.87	Joback Method
cpg	371.55	J/mol×K	655.62	Joback Method
cpg	381.42	J/mol×K	686.38	Joback Method
cpg	390.80	J/mol×K	717.13	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=R643435&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R643435&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>
<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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