

# Bicyclo[2.2.1]heptan-2-ol, 1,5,5-trimethyl-

<b>Other names:</b>	Isofenchol
<b>Inchi:</b>	InChI=1S/C10H18O/c1-9(2)6-10(3)5-7(9)4-8(10)11/h7-8,11H,4-6H2,1-3H3
<b>InchiKey:</b>	QNNGNRWQCQDOMF-UHFFFAOYSA-N
<b>Formula:</b>	C10H18O
<b>SMILES:</b>	CC1(C)CC2(C)CC1CC2O
<b>Mol. weight [g/mol]:</b>	154.25
<b>CAS:</b>	6168-62-3

## Physical Properties

Property code	Value	Unit	Source
gf	-20.50	kJ/mol	Joback Method
hf	-272.72	kJ/mol	Joback Method
hfus	9.46	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1114.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	529.27	K	Joback Method
tc	730.21	K	Joback Method
tf	334.96	K	Joback Method
vc	0.514	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.30	J/mol×K	529.27	Joback Method
cpg	370.25	J/mol×K	562.76	Joback Method
cpg	385.05	J/mol×K	596.25	Joback Method
cpg	398.92	J/mol×K	629.74	Joback Method
cpg	412.02	J/mol×K	663.23	Joback Method
cpg	424.55	J/mol×K	696.72	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=C6168623&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6168623&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>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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