

# Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-

<b>Other names:</b>	Carane Carane, cis
<b>Inchi:</b>	InChI=1S/C10H18/c1-7-4-5-8-9(6-7)10(8,2)3/h7-9H,4-6H2,1-3H3
<b>InchiKey:</b>	BWRHOYDPVJPXMF-UHFFFAOYSA-N
<b>Formula:</b>	C10H18
<b>SMILES:</b>	CC1CCC2C(C1)C2(C)C
<b>Mol. weight [g/mol]:</b>	138.25
<b>CAS:</b>	554-59-6

## Physical Properties

Property code	Value	Unit	Source
gf	121.81	kJ/mol	Joback Method
hf	-135.73	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	36.08	kJ/mol	Joback Method
ie	8.84	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	436.85	K	Joback Method
tc	642.10	K	Joback Method
tf	250.24	K	Joback Method
vc	0.497	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.02	J/molxK	436.85	Joback Method
cpg	307.28	J/molxK	471.06	Joback Method
cpg	326.14	J/molxK	505.27	Joback Method
cpg	343.70	J/molxK	539.47	Joback Method
cpg	360.10	J/molxK	573.68	Joback Method

cpg	375.46	J/mol×K	607.89	Joback Method
cpg	389.91	J/mol×K	642.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C554596&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C554596&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>
<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>

## 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>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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>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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