

# (Z) 2,3-Di-tert-butyl-2-butene

<b>Inchi:</b>	InChI=1S/C12H24/c1-9(11(3,4)5)10(2)12(6,7)8/h1-8H3/b10-9-
<b>InchiKey:</b>	UKVHFKANOLLXHC-KTKRTIGZSA-N
<b>Formula:</b>	C12H24
<b>SMILES:</b>	CC(=C(C)C(C)(C)C)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	168.32
<b>CAS:</b>	54429-93-5

## Physical Properties

Property code	Value	Unit	Source
gf	118.96	kJ/mol	Joback Method
hf	-123.10	kJ/mol	NIST Webbook
hfus	9.59	kJ/mol	Joback Method
hvap	39.83	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.415		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
tb	471.42	K	Joback Method
tc	667.75	K	Joback Method
tf	196.84	K	Joback Method
vc	0.667	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.10	J/molxK	471.42	Joback Method
cpg	415.17	J/molxK	504.14	Joback Method
cpg	434.03	J/molxK	536.86	Joback Method
cpg	451.74	J/molxK	569.58	Joback Method
cpg	468.37	J/molxK	602.31	Joback Method
cpg	483.99	J/molxK	635.03	Joback Method
cpg	498.67	J/molxK	667.75	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54429935&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54429935&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>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>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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