

# «beta»-Neoclovene

<b>Inchi:</b>	InChI=1S/C15H24/c1-11-6-5-8-14(4)12-7-9-15(11,14)10-13(12,2)3/h12H,1,5-10H2,2-4H3
<b>InchiKey:</b>	BUDWHMNUSAOQBI-UHFFFAOYSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	<chem>C=C1CCCC2(C)C3CCC12CC3(C)C</chem>
<b>Mol. weight [g/mol]:</b>	204.35
<b>CAS:</b>	56684-96-9

## Physical Properties

Property code	Value	Unit	Source
gf	262.37	kJ/mol	Joback Method
hf	-37.23	kJ/mol	Joback Method
hfus	5.83	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
tb	566.57	K	Joback Method
tc	800.20	K	Joback Method
tf	386.73	K	Joback Method
vc	0.708	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.14	J/molxK	566.57	Joback Method
cpg	522.76	J/molxK	605.51	Joback Method
cpg	543.69	J/molxK	644.45	Joback Method
cpg	563.39	J/molxK	683.38	Joback Method
cpg	582.28	J/molxK	722.32	Joback Method
cpg	600.82	J/molxK	761.26	Joback Method
cpg	619.44	J/molxK	800.20	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56684969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56684969&amp;Units=SI</a>
<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>

# 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

Latest version available from:

<https://www.chemeo.com/cid/14-104-0/beta-Neoclovene.pdf>

Generated by Cheméo on 2024-04-25 18:06:34.627962912 +0000 UTC m=+16357643.548540250.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.