

# (E)-Calamenene

<b>Inchi:</b>	InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9-10,12-13H,6,8H2
<b>InchiKey:</b>	PGTJIOWQJWHTJJ-OLZOCXBDSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	<chem>Cc1ccc2c(c1)C(C(C)C)CCC2C</chem>
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	207.07	kJ/mol	Joback Method
hf	-98.32	kJ/mol	Joback Method
hfus	21.45	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.632		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1516.00		NIST Webbook
tb	585.14	K	Joback Method
tc	803.63	K	Joback Method
tf	305.45	K	Joback Method
vc	0.710	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.92	J/molxK	585.14	Joback Method
cpg	503.81	J/molxK	621.55	Joback Method
cpg	523.46	J/molxK	657.97	Joback Method
cpg	541.93	J/molxK	694.38	Joback Method
cpg	559.26	J/molxK	730.80	Joback Method
cpg	575.50	J/molxK	767.21	Joback Method
cpg	590.72	J/molxK	803.63	Joback Method
dvisc	0.0018212	Paxs	305.45	Joback Method
dvisc	0.0011104	Paxs	352.07	Joback Method

dvisc	0.0007601	Paxs	398.68	Joback Method
dvisc	0.0005632	Paxs	445.30	Joback Method
dvisc	0.0004418	Paxs	491.91	Joback Method
dvisc	0.0003614	Paxs	538.52	Joback Method
dvisc	0.0003052	Paxs	585.14	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R616889&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R616889&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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

Latest version available from:

<https://www.chemeo.com/cid/79-053-6/E-Calamenene.pdf>

Generated by Cheméo on 2024-04-25 21:48:00.603671399 +0000 UTC m=+16370929.524248746.

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