

# Calamene

<b>Inchi:</b>	InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h6,8,10-11H,5,7,9H2,1-4
<b>InchiKey:</b>	LVIDDMJSLAVTSZ-UHFFFAOYSA-N
<b>Formula:</b>	C15H22
<b>SMILES:</b>	Cc1ccc(C(C)C)c2c1CCC(C)C2
<b>Mol. weight [g/mol]:</b>	202.34

## Physical Properties

Property code	Value	Unit	Source
gf	205.15	kJ/mol	Joback Method
hf	-89.45	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.243		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1523.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	594.79	K	Joback Method
tc	814.30	K	Joback Method
tf	322.21	K	Joback Method
vc	0.711	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.12	J/molxK	594.79	Joback Method
cpg	571.28	J/molxK	777.72	Joback Method
cpg	555.62	J/molxK	741.13	Joback Method
cpg	538.92	J/molxK	704.55	Joback Method
cpg	521.14	J/molxK	667.96	Joback Method
cpg	502.23	J/molxK	631.38	Joback Method
cpg	585.98	J/molxK	814.30	Joback Method
dvisc	0.0002663	Paxs	594.79	Joback Method

dvisc	0.0003208	Paxs	549.36	Joback Method
dvisc	0.0003995	Paxs	503.93	Joback Method
dvisc	0.0005197	Paxs	458.50	Joback Method
dvisc	0.0007164	Paxs	413.07	Joback Method
dvisc	0.0010690	Paxs	367.64	Joback Method
dvisc	0.0017856	Paxs	322.21	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R633151&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R633151&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>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/74-955-0/Calamene.pdf>

Generated by Cheméo on 2024-04-27 16:52:39.344087405 +0000 UTC m=+16526008.264664720.

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