

# «alpha»-Calacorene

<b>Other names:</b>	1-Isopropyl-4,7-dimethyl-1,2-dihydronaphthalene, (S)- «alpha»-Calacorene, (+)- Cadina-1,3,5,9-tetraene (E)-Calacorene «alpha»-Colocarene
<b>Inchi:</b>	InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5-7,9-10,13H,8H2,1-4H
<b>InchiKey:</b>	CUUMXRBKJIDIAY-UHFFFAOYSA-N
<b>Formula:</b>	C15H20
<b>SMILES:</b>	CC1=CCC(C(C)C)c2cc(C)ccc21
<b>Mol. weight [g/mol]:</b>	200.32
<b>CAS:</b>	21391-99-1

## Physical Properties

Property code	Value	Unit	Source
gf	235.11	kJ/mol	Joback Method
hf	-31.67	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.542		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1542.00		NIST Webbook
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# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.53	J/molxK	593.95	Joback Method
cpg	545.52	J/molxK	778.60	Joback Method
cpg	530.81	J/molxK	741.67	Joback Method
cpg	515.11	J/molxK	704.74	Joback Method
cpg	498.37	J/molxK	667.81	Joback Method
cpg	480.53	J/molxK	630.88	Joback Method
cpg	559.31	J/molxK	815.53	Joback Method
dvisc	0.0002728	Paxs	593.95	Joback Method
dvisc	0.0003240	Paxs	548.79	Joback Method
dvisc	0.0003969	Paxs	503.62	Joback Method
dvisc	0.0005061	Paxs	458.46	Joback Method
dvisc	0.0006804	Paxs	413.30	Joback Method
dvisc	0.0009838	Paxs	368.13	Joback Method
dvisc	0.0015769	Paxs	322.97	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21391991&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21391991&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>ripol:</b>	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

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