

# «beta»-Calacorene

<b>Inchi:</b>	InChI=1S/C15H20/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9,12H,6,8H2,1-4H3
<b>InchiKey:</b>	HDBSITBZJGRUAD-UHFFFAOYSA-N
<b>Formula:</b>	C15H20
<b>SMILES:</b>	CC(C)=C1CCC(C)c2ccc(C)cc21
<b>Mol. weight [g/mol]:</b>	200.32

## Physical Properties

Property code	Value	Unit	Source
gf	254.13	kJ/mol	Joback Method
hf	-6.46	kJ/mol	Joback Method
hfus	22.92	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.686		Crippen Method
mcvol	183.290	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1563.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1564.00		NIST Webbook
ripol	1942.00		NIST Webbook
tb	596.77	K	Joback Method
tc	821.36	K	Joback Method
tf	321.09	K	Joback Method
vc	0.701	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.34	J/molxK	596.77	Joback Method
cpg	480.53	J/molxK	634.20	Joback Method
cpg	498.53	J/molxK	671.63	Joback Method
cpg	515.41	J/molxK	709.06	Joback Method
cpg	531.24	J/molxK	746.49	Joback Method
cpg	546.07	J/molxK	783.93	Joback Method
cpg	559.99	J/molxK	821.36	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R604836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R604836&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>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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