

# epi-«beta»-Cadinol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h10,12-14,16H,3,5-
<b>InchiKey:</b>	DCGIIRVFKWJQME-APIJFGDWSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	<chem>C=C1CCC2C(C1)C(C(C)C)CCC2(C)O</chem>
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-330.68	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	654.96	K	Joback Method
tc	859.10	K	Joback Method
tf	355.53	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.74	J/mol×K	654.96	Joback Method
cpg	616.91	J/mol×K	688.98	Joback Method
cpg	636.06	J/mol×K	723.01	Joback Method
cpg	654.29	J/mol×K	757.03	Joback Method
cpg	671.72	J/mol×K	791.05	Joback Method
cpg	688.46	J/mol×K	825.08	Joback Method
cpg	704.61	J/mol×K	859.10	Joback Method

# Sources

<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=R442054&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R442054&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpola:</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

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