

# Cadinan-3-«beta»,10-«beta»-diol

<b>Inchi:</b>	InChI=1S/C15H28O2/c1-9(2)11-5-6-15(4,17)13-8-14(16)10(3)7-12(11)13/h9-14,16-17H,5
<b>InchiKey:</b>	OSZJZKFYUTYGQX-GBGJHRCWSA-N
<b>Formula:</b>	C15H28O2
<b>SMILES:</b>	CC(C)C1CCC(C)(O)C2CC(O)C(C)CC12
<b>Mol. weight [g/mol]:</b>	240.38

## Physical Properties

Property code	Value	Unit	Source
gf	-163.89	kJ/mol	Joback Method
hf	-607.83	kJ/mol	Joback Method
hfus	25.12	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.827		Crippen Method
mcvol	212.230	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinsol	1740.00		NIST Webbook
tb	738.64	K	Joback Method
tc	932.18	K	Joback Method
tf	394.19	K	Joback Method
vc	0.783	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.60	J/molxK	738.64	Joback Method
cpg	717.17	J/molxK	770.90	Joback Method
cpg	734.95	J/molxK	803.15	Joback Method
cpg	752.03	J/molxK	835.41	Joback Method
cpg	768.50	J/molxK	867.67	Joback Method
cpg	784.45	J/molxK	899.93	Joback Method
cpg	799.98	J/molxK	932.18	Joback Method

# Sources

<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=R391525&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R391525&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>

# 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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