

# Calarane

**Inchi:** InChI=1S/C15H26/c1-10-6-5-7-11-8-9-12-13(14(12,2)3)15(10,11)4/h10-13H,5-9H2,1-4H3  
**InchiKey:** MKGHZTWCWRGKCY-HHQTALHSA-N  
**Formula:** C15H26  
**SMILES:** CC1CCCC2CCC3C(C3(C)C)C12C  
**Mol. weight [g/mol]:** 206.37

## Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	-177.39	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.495		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
ripol	1489.00		NIST Webbook
ripol	1508.00		NIST Webbook
ripol	1489.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1670.00		NIST Webbook
tb	557.83	K	Joback Method
tc	780.06	K	Joback Method
tf	340.67	K	Joback Method
vc	0.724	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	557.83	Joback Method
cpg	547.59	J/mol×K	594.87	Joback Method
cpg	570.94	J/mol×K	631.91	Joback Method
cpg	592.86	J/mol×K	668.95	Joback Method
cpg	613.64	J/mol×K	705.99	Joback Method

cpg	633.54	J/mol×K	743.02	Joback Method
cpg	652.86	J/mol×K	780.06	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=R134184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R134184&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>

## 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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