

# «alpha»-Maaliene

<b>Inchi:</b>	InChI=1S/C15H24/c1-10-6-5-8-15(4)9-7-11-13(12(10)15)14(11,2)3/h6,11-13H,5,7-9H2,1
<b>InchiKey:</b>	OULROVQTHHSDPX-UHFFFAOYSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC1=CCCC2(C)CCC3C(C12)C3(C)C
<b>Mol. weight [g/mol]:</b>	204.35
<b>CAS:</b>	489-28-1

## Physical Properties

Property code	Value	Unit	Source
gf	227.40	kJ/mol	Joback Method
hf	-110.74	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mvol	185.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1442.70		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	566.64	K	Joback Method
tc	792.17	K	Joback Method
tf	358.19	K	Joback Method
vc	0.711	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/mol×K	566.64	Joback Method
cpg	526.55	J/mol×K	604.23	Joback Method
cpg	547.97	J/mol×K	641.82	Joback Method
cpg	568.10	J/mol×K	679.41	Joback Method
cpg	587.25	J/mol×K	716.99	Joback Method
cpg	605.70	J/mol×K	754.58	Joback Method
cpg	623.74	J/mol×K	792.17	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C489281&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C489281&amp;Units=SI</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>hvp:</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>rinp:</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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