

# Alismol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10(2)12-6-5-11(3)13-7-8-15(4,16)14(13)9-12/h9-10,13-14,16H,3,
<b>InchiKey:</b>	BUPJOLXWQXEJSQ-ZNMIVQPWSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	<chem>C=C1CCC(C(C)C)=CC2C1CCC2(C)O</chem>
<b>Mol. weight [g/mol]:</b>	220.35
<b>CAS:</b>	87827-55-2

## Physical Properties

Property code	Value	Unit	Source
gf	69.47	kJ/mol	Joback Method
hf	-264.03	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1619.00		NIST Webbook
rinpol	1620.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2260.00		NIST Webbook
ripol	2272.00		NIST Webbook
tb	663.77	K	Joback Method
tc	870.50	K	Joback Method
tf	373.05	K	Joback Method
vc	0.738	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/molxK	663.77	Joback Method
cpg	590.64	J/molxK	698.22	Joback Method
cpg	608.29	J/molxK	732.68	Joback Method
cpg	625.13	J/molxK	767.13	Joback Method

cpg	641.29	J/mol×K	801.59	Joback Method
cpg	656.87	J/mol×K	836.04	Joback Method
cpg	671.99	J/mol×K	870.50	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=C87827552&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C87827552&amp;Units=SI</a>
<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>

## 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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