

# Spirojatamol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-11(2)13-7-6-12(3)15(10-13)9-5-8-14(15,4)16/h11,13,16H,3,5-10H
<b>InchiKey:</b>	AEUBOEQPIBOTGP-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	<chem>C=C1CCC(C(C)C)CC12CCCC2(C)O</chem>
<b>Mol. weight [g/mol]:</b>	222.37
<b>CAS:</b>	128487-46-7

## Physical Properties

Property code	Value	Unit	Source
gf	43.65	kJ/mol	Joback Method
hf	-295.10	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1592.10		NIST Webbook
rinpol	1592.10		NIST Webbook
tb	659.87	K	Joback Method
tc	871.10	K	Joback Method
tf	383.67	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.59	J/mol×K	659.87	Joback Method
cpg	611.26	J/mol×K	695.07	Joback Method
cpg	630.08	J/mol×K	730.28	Joback Method
cpg	648.26	J/mol×K	765.48	Joback Method
cpg	666.01	J/mol×K	800.69	Joback Method
cpg	683.54	J/mol×K	835.89	Joback Method
cpg	701.06	J/mol×K	871.10	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=C128487467&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C128487467&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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