

# Guaioxide

<b>Inchi:</b>	InChI=1S/C15H26O/c1-10-5-7-12-9-15(16-14(12,3)4)11(2)6-8-13(10)15/h10-13H,5-9H2,
<b>InchiKey:</b>	GXMJXGUEPXEOGR-IPNSXDPFSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC1CCC2CC3(OC2(C)C)C(C)CCC13
<b>Mol. weight [g/mol]:</b>	222.37
<b>CAS:</b>	20149-50-2

## Physical Properties

Property code	Value	Unit	Source
gf	101.14	kJ/mol	Joback Method
hf	-315.55	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	50.52	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.016		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1516.00		NIST Webbook
ripol	1697.00		NIST Webbook
ripol	1697.00		NIST Webbook
tb	589.05	K	Joback Method
tc	816.69	K	Joback Method
tf	363.72	K	Joback Method
vc	0.737	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/molxK	589.05	Joback Method
cpg	586.42	J/molxK	626.99	Joback Method
cpg	609.68	J/molxK	664.93	Joback Method
cpg	631.66	J/molxK	702.87	Joback Method
cpg	652.64	J/molxK	740.81	Joback Method

cpg	672.91	J/mol×K	778.75	Joback Method
cpg	692.75	J/mol×K	816.69	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=C20149502&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20149502&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>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>ripola:</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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