

# 15-nor-Funebran-3-one

<b>Inchi:</b>	InChI=1S/C14H22O/c1-9-4-5-12-13(2,3)10-8-14(9,12)7-6-11(10)15/h9-10,12H,4-8H2,1-3
<b>InchiKey:</b>	LHRXTEZLJOREFX-QTQSFLCGSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC1CCC2C(C)(C)C3CC12CCC3=O
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	76.06	kJ/mol	Joback Method
hf	-274.11	kJ/mol	Joback Method
hfus	11.28	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.428		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1599.00		NIST Webbook
rinpol	1562.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2150.00		NIST Webbook
tb	607.44	K	Joback Method
tc	847.85	K	Joback Method
tf	401.86	K	Joback Method
vc	0.675	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.23	J/molxK	607.44	Joback Method
cpg	534.02	J/molxK	647.51	Joback Method
cpg	555.46	J/molxK	687.58	Joback Method
cpg	575.85	J/molxK	727.65	Joback Method

cpg	595.52	J/mol×K	767.72	Joback Method
cpg	614.78	J/mol×K	807.79	Joback Method
cpg	633.95	J/mol×K	847.85	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=R198702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R198702&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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