

# 15-nor-Prezizaan-7-one

<b>Inchi:</b>	InChI=1S/C13H18O/c1-8-3-4-11-12(14)9(2)10-5-6-13(8,11)7-10/h8,10-11H,2-7H2,1H3/t8
<b>InchiKey:</b>	PSJUKNBMBYBQSO-FSWKUEMBSA-N
<b>Formula:</b>	C13H18O
<b>SMILES:</b>	<chem>C=C1C(=O)C2CCC(C)C23CCC1C3</chem>
<b>Mol. weight [g/mol]:</b>	190.28

## Physical Properties

Property code	Value	Unit	Source
gf	133.92	kJ/mol	Joback Method
hf	-164.13	kJ/mol	Joback Method
hfus	12.75	kJ/mol	Joback Method
hvap	47.56	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.958		Crippen Method
mcvol	158.720	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1572.00		NIST Webbook
ripol	2035.00		NIST Webbook
tb	588.15	K	Joback Method
tc	825.95	K	Joback Method
tf	384.61	K	Joback Method
vc	0.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.44	J/molxK	588.15	Joback Method
cpg	459.22	J/molxK	627.78	Joback Method
cpg	478.64	J/molxK	667.42	Joback Method
cpg	496.89	J/molxK	707.05	Joback Method
cpg	514.16	J/molxK	746.68	Joback Method
cpg	530.65	J/molxK	786.32	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=R198717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R198717&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.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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