

# Prezizaan-15-aI

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10-4-5-13-14(2,3)12(9-16)11-6-7-15(10,13)8-11/h9-13H,4-8H2,1-
<b>InchiKey:</b>	FHSLAXWYMZHYPS-BRUFJSJZSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC1CCC2C(C)(C)C(C=O)C3CCC12C3
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	99.84	kJ/mol	Joback Method
hf	-262.97	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	52.56	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.674		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1663.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1660.00		NIST Webbook
ripol	2155.00		NIST Webbook
ripol	2155.00		NIST Webbook
tb	606.49	K	Joback Method
tc	831.12	K	Joback Method
tf	382.67	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.11	J/molxK	606.49	Joback Method
cpg	575.51	J/molxK	643.93	Joback Method
cpg	596.54	J/molxK	681.37	Joback Method

cpg	616.51	J/mol×K	718.81	Joback Method
cpg	635.69	J/mol×K	756.25	Joback Method
cpg	654.37	J/mol×K	793.69	Joback Method
cpg	672.85	J/mol×K	831.12	Joback Method

## Sources

<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=R199250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R199250&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>

## 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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