

# Tricyclo[3.2.1.0<sup>2,4</sup>]octan-8-one,exo-

<b>Inchi:</b>	InChI=1S/C8H12/c1-2-6-3-5(1)7-4-8(6)7/h5-8H,1-4H2/t5?,6?,7-,8+
<b>InchiKey:</b>	PSZPCAFRANQPLS-HYNHDVCUSA-N
<b>Formula:</b>	C8H10O
<b>SMILES:</b>	C1CC2CC1C1CC21
<b>Mol. weight [g/mol]:</b>	122.16
<b>CAS:</b>	7076-83-7

## Physical Properties

Property code	Value	Unit	Source
gf	203.12	kJ/mol	Joback Method
hf	-4.23	kJ/mol	Joback Method
hfus	14.05	kJ/mol	Joback Method
hvap	32.66	kJ/mol	Joback Method
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mcvol	91.000	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	393.72	K	Joback Method
tc	594.92	K	Joback Method
tf	233.02	K	Joback Method
vc	0.361	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.89	J/mol×K	393.72	Joback Method
cpg	204.36	J/mol×K	427.25	Joback Method
cpg	220.54	J/mol×K	460.79	Joback Method
cpg	235.52	J/mol×K	494.32	Joback Method
cpg	249.40	J/mol×K	527.85	Joback Method
cpg	262.25	J/mol×K	561.38	Joback Method
cpg	274.16	J/mol×K	594.92	Joback Method
dvisc	0.0001567	Paxs	233.02	Joback Method

dvisc	0.0002381	Paxs	259.80	Joback Method
dvisc	0.0003344	Paxs	286.59	Joback Method
dvisc	0.0004433	Paxs	313.37	Joback Method
dvisc	0.0005621	Paxs	340.15	Joback Method
dvisc	0.0006884	Paxs	366.94	Joback Method
dvisc	0.0008202	Paxs	393.72	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=C7076837&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7076837&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>ie:</b>	Ionization energy
<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>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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