

# 7-Oxy-6, 8-dioxabicyclo-(3,2,1) - octane

<b>Other names:</b>	7,8-dioxabicyclo[3.2.1]octan-6-one
<b>Inchi:</b>	InChI=1S/C6H8O3/c7-6-4-2-1-3-5(8-4)9-6/h4-5H,1-3H2
<b>InchiKey:</b>	FDTQYEHORIQWRC-UHFFFAOYSA-N
<b>Formula:</b>	C6H8O3
<b>SMILES:</b>	O=C1OC2CCCC1O2
<b>Mol. weight [g/mol]:</b>	128.13
<b>CAS:</b>	5257-20-5

## Physical Properties

Property code	Value	Unit	Source
gf	-197.89	kJ/mol	Joback Method
hf	-435.59	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.438		Crippen Method
mcvol	86.990	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	480.42	K	Joback Method
tc	714.56	K	Joback Method
tf	307.58	K	Joback Method
vc	0.319	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.75	J/molxK	480.42	Joback Method
cpg	219.61	J/molxK	519.44	Joback Method
cpg	232.64	J/molxK	558.47	Joback Method
cpg	244.87	J/molxK	597.49	Joback Method
cpg	256.33	J/molxK	636.51	Joback Method
cpg	267.03	J/molxK	675.54	Joback Method
cpg	277.00	J/molxK	714.56	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=C5257205&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5257205&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>

# 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>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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