

# 1,8-cineol-5-one

<b>Inchi:</b>	InChI=1S/C10H16O2/c1-9(2)7-4-5-10(3,12-9)6-8(7)11/h7H,4-6H2,1-3H3
<b>InchiKey:</b>	RFXTXEOQEMTRHL-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O2
<b>SMILES:</b>	CC12CCC(C(=O)C1)C(C)(C)O2
<b>Mol. weight [g/mol]:</b>	168.23

## Physical Properties

Property code	Value	Unit	Source
gf	-96.78	kJ/mol	Joback Method
hf	-376.01	kJ/mol	Joback Method
hfus	9.69	kJ/mol	Joback Method
hvap	44.17	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.923		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinqol	1206.00		NIST Webbook
tb	540.80	K	Joback Method
tc	780.01	K	Joback Method
tf	369.65	K	Joback Method
vc	0.516	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.06	J/mol×K	540.80	Joback Method
cpg	374.39	J/mol×K	580.67	Joback Method
cpg	391.40	J/mol×K	620.54	Joback Method
cpg	407.37	J/mol×K	660.41	Joback Method
cpg	422.55	J/mol×K	700.27	Joback Method
cpg	437.20	J/mol×K	740.14	Joback Method
cpg	451.60	J/mol×K	780.01	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R320924&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R320924&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.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>

# 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>rinpola:</b>	Non-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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