

# 2,4,6-Cycloheptatrien-1-one, 2-hydroxy-

<b>Other names:</b>	Tropolone Purpurocatechol 2-Hydroxy-2,4,6-cycloheptatriene-1-one 2-Hydroxy-2,4,6-cycloheptatrien-1-one 2-hydroxycyclohepta-2,4,6-trienone
<b>Inchi:</b>	InChI=1S/C7H6O2/c8-6-4-2-1-3-5-7(6)9/h1-5H,(H,8,9)
<b>InchiKey:</b>	MDYOLVRUBBJPFM-UHFFFAOYSA-N
<b>Formula:</b>	C7H6O2
<b>SMILES:</b>	O=c1cccc1O
<b>Mol. weight [g/mol]:</b>	122.12
<b>CAS:</b>	533-75-5

## Physical Properties

Property code	Value	Unit	Source
chs	-3372.60	kJ/mol	NIST Webbook
chs	-3382.00 ± 2.00	kJ/mol	NIST Webbook
chs	-3370.00	kJ/mol	NIST Webbook
chs	-3373.00 ± 4.00	kJ/mol	NIST Webbook
hf	-156.00 ± 1.00	kJ/mol	NIST Webbook
hf	-155.00	kJ/mol	NIST Webbook
hfs	-239.00	kJ/mol	NIST Webbook
hfs	-239.70 ± 2.60	kJ/mol	NIST Webbook
hfs	-239.50 ± 0.80	kJ/mol	NIST Webbook
hsub	83.70 ± 0.80	kJ/mol	NIST Webbook
hsub	83.70 ± 0.80	kJ/mol	NIST Webbook
hsub	83.70 ± 0.80	kJ/mol	NIST Webbook
ie	9.86 ± 0.02	eV	NIST Webbook
log10ws	-0.44		Crippen Method
logp	0.752		Crippen Method
mvol	93.170	ml/mol	McGowan Method
ripol	2003.00		NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	84.10 ± 0.40	kJ/mol	297.00	NIST Webbook
hsubt	84.10 ± 0.40	kJ/mol	303.00	NIST Webbook

## Sources

<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>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=C533755&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C533755&amp;Units=SI</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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>ripol:</b>	Polar retention indices

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