

# 9H-Xanthen-9-ol, 9-phenyl-

<b>Other names:</b>	3-chloro-2,3-dimethylpentane 9-Phenyl-9-xanthenol 9-Phenylxanthen-9-ol
<b>Inchi:</b>	InChI=1S/C19H14O2/c20-19(14-8-2-1-3-9-14)15-10-4-6-12-17(15)21-18-13-7-5-11-16(18)
<b>InchiKey:</b>	CVZUPKFPOSRRSK-UHFFFAOYSA-N
<b>Formula:</b>	C7H15Cl
<b>SMILES:</b>	OC1(c2ccccc2)c2ccccc2Oc2ccccc21
<b>Mol. weight [g/mol]:</b>	134.65
<b>CAS:</b>	596-38-3

## Physical Properties

Property code	Value	Unit	Source
gf	271.49	kJ/mol	Joback Method
hf	61.13	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.076		Crippen Method
mcvol	208.170	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	845.96	K	Joback Method
tc	1098.62	K	Joback Method
tf	540.94	K	Joback Method
vc	0.778	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.32	J/mol×K	845.96	Joback Method
cpg	621.15	J/mol×K	888.07	Joback Method
cpg	635.98	J/mol×K	930.18	Joback Method
cpg	651.11	J/mol×K	972.29	Joback Method
cpg	666.85	J/mol×K	1014.40	Joback Method
cpg	683.48	J/mol×K	1056.51	Joback Method

cpg

701.30

J/mol×K

1098.62

Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32451e+01
Coeff. B	-3.21672e+03
Coeff. C	-5.26700e+01
Temperature range (K), min.	300.92
Temperature range (K), max.	458.12

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C596383&Units=SI>

**The Yaws Handbook of Vapor Pressure:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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