

# Benzeneacetaldehyde, «alpha»-phenyl-

<b>Other names:</b>	Acetaldehyde, diphenyl- Diphenylacetaldehyde Diphenylethanal 2,2-Diphenylacetaldehyde 2-Phenyl-benzeneacetaldehyde
<b>Inchi:</b>	InChI=1S/C14H12O/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-11,14H
<b>InchiKey:</b>	HLLGFGBLKOIZOM-UHFFFAOYSA-N
<b>Formula:</b>	C14H12O
<b>SMILES:</b>	O=CC(c1ccccc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	196.24
<b>CAS:</b>	947-91-1

## Physical Properties

Property code	Value	Unit	Source
gf	189.86	kJ/mol	Joback Method
hf	49.91	kJ/mol	Joback Method
hfus	18.86	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.017		Crippen Method
mcvol	162.170	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	588.20	K	NIST Webbook
tc	867.81	K	Joback Method
tf	327.38	K	Joback Method
vc	0.615	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.00	J/molxK	621.30	Joback Method
cpg	458.93	J/molxK	826.73	Joback Method
cpg	447.85	J/molxK	785.64	Joback Method
cpg	435.70	J/molxK	744.56	Joback Method

cpg	422.40	J/molxK	703.47	Joback Method
cpg	407.86	J/molxK	662.39	Joback Method
cpg	469.03	J/molxK	867.81	Joback Method
dvisc	0.0001946	Paxs	621.30	Joback Method
dvisc	0.0002537	Paxs	572.31	Joback Method
dvisc	0.0003476	Paxs	523.33	Joback Method
dvisc	0.0005084	Paxs	474.34	Joback Method
dvisc	0.0008115	Paxs	425.35	Joback Method
dvisc	0.0014629	Paxs	376.37	Joback Method
dvisc	0.0031460	Paxs	327.38	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C947911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C947911&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>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>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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