

Benzeneacetaldehyde, «alpha»-phenyl-

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

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=C947911&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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