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]: 196.25

Physical Properties

Property code	Value	Unit	Source
af	0.4327		Cheméo Relay (1.0)
gf	189.86	kJ/mol	Joback Method
hf	66.68	kJ/mol	Cheméo Relay (1.0)
hfus	18.86	kJ/mol	Joback Method
hvap	68.13	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-3.45		Cheméo Relay (1.0)
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	842.85	K	Cheméo Relay (1.0)
tf	345.80	K	Cheméo Relay (1.0)
vc	0.570	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.00	J/mol×K	621.30	Joback Method
cpg	469.03	J/mol×K	867.81	Joback Method
cpg	458.93	J/mol×K	826.73	Joback Method

cpg	447.85	J/mol×K	785.64	Joback Method
cpg	435.70	J/mol×K	744.56	Joback Method
cpg	422.40	J/mol×K	703.47	Joback Method
cpg	407.86	J/mol×K	662.39	Joback Method
dvisc	0.0005084	Pa×s	474.34	Joback Method
dvisc	0.0001946	Pa×s	621.30	Joback Method
dvisc	0.0002537	Pa×s	572.31	Joback Method
dvisc	0.0003476	Pa×s	523.33	Joback Method
dvisc	0.0031460	Pa×s	327.38	Joback Method
dvisc	0.0008115	Pa×s	425.35	Joback Method
dvisc	0.0014629	Pa×s	376.37	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C947911&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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