Benzilic acid

Other names:	2,2-Diphenyl-2-hydroxyacetic acid
	2-Hydroxy-2,2-diphenylacetic acid
	Acide diphenylhydroxyacetique
	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-
	Benzeneacetic acid, Â«alphaÂ»-hydroxy-Â«alphaÂ»-phenyl-
	Benzylic acid
	Diphenylglycolic acid
	Diphenylhydroxyacetic acid
	Glycolic acid, diphenyl-
	Hydroxydiphenylacetic acid
	Mandelic acid, «alpha»-phenyl-
	Mandelic acid, Â«alphaÂ»-phenyl-
	NSC 2830
	«alpha»,«alpha»-Diphenyl-«alpha»-hydroxyacetic acid
	«alpha»,«alpha»-Diphenylglycolic acid
	«alpha»-Hydroxy-2,2-diphenylacetic acid
	«alpha»-Hydroxy-«alpha»-phenylbenzeneacetic acid
	«alpha»-Hydroxydiphenylacetic acid
	Â«alphaÂ»,Â«alphaÂ»-Diphenyl-Â«alphaÂ»-hydroxyacetic acid
	Â«alphaÂ»,Â«alphaÂ»-Diphenylglycolic acid
	Â«alphaÂ»-Hydroxy-2,2-diphenylacetic acid
	Â«alphaÂ»-Hydroxy-Â«alphaÂ»-phenylbenzeneacetic acid
	Â«alphaÂ»-Hydroxydiphenylacetic acid
Inchi:	InChI=1S/C14H12O3/c15-13(16)14(17,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,17H,(H,1
InchiKey:	UKXSKSHDVLQNKG-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	O=C(O)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	228.24
CAS:	76-93-7

Physical Properties

Property code	Value	Unit	Source
gf	-107.90	kJ/mol	Joback Method
hf	-285.02	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	90.12	kJ/mol	Joback Method

log10ws	-2.21		Aqueous Solubility Prediction Method
logp	2.007		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	808.08	K	Joback Method
tc	1029.71	K	Joback Method
tf	423.52	K	Aqueous Solubility Prediction Method
tf	423.00 ± 3.00	K	NIST Webbook
tf	422.00 ± 3.00	K	NIST Webbook
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.32	J/mol×K	808.08	Joback Method
cpg	531.07	J/mol×K	992.77	Joback Method
cpg	524.11	J/mol×K	955.83	Joback Method
cpg	516.64	J/mol×K	918.89	Joback Method
cpg	508.58	J/mol×K	881.96	Joback Method
cpg	499.84	J/mol×K	845.02	Joback Method
cpg	537.61	J/mol×K	1029.71	Joback Method
dvisc	0.0000052	Pa×s	808.08	Joback Method
dvisc	0.0000087	Pa×s	752.46	Joback Method
dvisc	0.0000158	Pa×s	696.84	Joback Method
dvisc	0.0000317	Pa×s	641.23	Joback Method
dvisc	0.0000730	Pa×s	585.61	Joback Method
dvisc	0.0001999	Pa×s	529.99	Joback Method
dvisc	0.0006931	Pa×s	474.37	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76937&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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