Benzoin

Other names:	(.+/-.)-Benzoin
	.alpha.-hydroxy-.alpha.-phenylacetophenone
	1,2-diphenyl-2-hydroxyethanone
	2-Hydroxy-1,2-diphenylethan-1-one
	2-Hydroxy-1,2-diphenylethanone
	2-Hydroxy-2-phenylacetophenone
	Acetophenone, 2-hydroxy-2-phenyl-
	Benzoylphenylcarbinol
	Bitter almond oil camphor
	Ethanone, 2-hydroxy-1,2-diphenyl-
	Fenyl-«alpha»-hydroxybenzylketon
	Fenyl-Â«alphaÂ»-hydroxybenzylketon
	Ketone, «alpha»-hydroxybenzyl phenyl
	Ketone, Â«alphaÂ»-hydroxybenzyl phenyl
	NCI-C50011
	NSC 8082
	Phenyl-«alpha»-hydroxybenzyl ketone
	Phenyl-Â«alphaÂ»-hydroxybenzyl ketone
	Wy 42956
	ethanone, 2-hydroxyl-1,2-diphenyl-
	«alpha»-Hydroxy-«alpha»-phenylacetophenone
	«alpha»-Hydroxybenzyl phenyl ketone
	Â«alphaÂ»-Hydroxy-Â«alphaÂ»-phenylacetophenone
	Â«alphaÂ»-Hydroxybenzyl phenyl ketone
Inchi:	InChI=1S/C14H12O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10,13,15H
InchiKey:	ISAOCJYIOMOJEB-UHFFFAOYSA-N
Formula:	C14H12O2
SMILES:	O=C(c1ccccc1)C(O)c1ccccc1
Mol. weight [g/mol]:	212.24
CAS:	119-53-9

Physical Properties

Property code	Value	Unit	Source
chs	-6976.00 ± 3.00	kJ/mol	NIST Webbook
gf	23.64	kJ/mol	Joback Method
hf	-129.32	kJ/mol	Joback Method

hfs	-247.90	kJ/mol	NIST Webbook
hfus	35.85	kJ/mol	Solubility of Benzoin in Six Monosolvents and in Some Binary Solvent Mixtures at Various Temperatures
hvap	74.35	kJ/mol	Joback Method
log10ws	-2.85		Estimated Solubility Method
log10ws	-3.23		Aqueous Solubility Prediction Method
logp	2.603		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	718.69	K	Joback Method
tc	948.69	K	Joback Method
tf	408.75	K	Aqueous Solubility Prediction Method
tf	408.00 ± 2.00	K	NIST Webbook
tf	406.50 ± 0.50	K	NIST Webbook
tf	407.00 ± 3.00	K	NIST Webbook
tf	406.00 ± 3.00	K	NIST Webbook
tt	410.90	K	Solubility Modeling and Mixing Properties for Benzoin in Different Monosolvents and Solvent Mixtures at the Temperature Range from 273.15 to 313.15 K
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.76	J/mol×K	718.69	Joback Method
cpg	455.12	J/mol×K	757.02	Joback Method
cpg	466.48	J/mol×K	795.36	Joback Method
cpg	476.88	J/mol×K	833.69	Joback Method
cpg	486.41	J/mol×K	872.02	Joback Method
cpg	495.13	J/mol×K	910.35	Joback Method
cpg	503.12	J/mol×K	948.69	Joback Method
dvisc	0.0026796	Pa×s	396.13	Joback Method
dvisc	0.0008779	Pa×s	449.89	Joback Method
dvisc	0.0003650	Pa×s	503.65	Joback Method
dvisc	0.0001797	Pa×s	557.41	Joback Method
dvisc	0.0001003	Pa×s	611.17	Joback Method

dvisc	0.0000615	Pa×s	664.93	Joback Method
dvisc	0.0000405	Pa×s	718.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	617.00	K	102.00	NIST Webbook
tbrp	467.00	K	1.60	NIST Webbook

Sources

Solubility Modeling and Mixing Properties for Benzoin in Different Monosolvents and Solvent Mixtures at the Temperature Range from 273.15 to 313.15 K:	https://www.doi.org/10.1021/acs.jced.7b00743
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119539&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determining the Solubility of Organic Compounds in Supercritical Carbon Dioxide Using Supercritical Fluid Chromatography Directly Interfaced to Supercritical Fluid Solubility Apparatus:	https://www.doi.org/10.1021/acs.jced.6b00081
Solubility of Benzoin in Six Monosolvents and in Some Binary Mixtures at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.7b00238
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume