Benzenemethanol, «alpha»-phenyl-

Other names:	.alpha.-phenylbenzenemethanol
	Benzhydrol
	Benzhydryl alcohol
	Benzohydrol
	Diphenylcarbinol
	Diphenylmethanol
	Diphenylmethyl alcohol
	Hydroxydiphenylmethane
	NSC 32150
	alpha-Phenylbenzenemethanol
	«alpha»-Phenylbenzenemethanol
	«alpha»-Phenylbenzyl alcohol
	Â«alphaÂ»-Phenylbenzenemethanol
	Â«alphaÂ»-Phenylbenzyl alcohol
Inchi:	InChI=1S/C13H12O/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10,13-14H
InchiKey:	QILSFLSDHQAZET-UHFFFAOYSA-N
Formula:	C13H12O
SMILES:	OC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	184.23
CAS:	91-01-0

Physical Properties

Property code	Value	Unit	Source
chs	-6725.45	kJ/mol	NIST Webbook
chs	-6752.60	kJ/mol	NIST Webbook
gf	144.14	kJ/mol	Joback Method
hf	3.90	kJ/mol	Joback Method
hfs	-105.30 ± 2.10	kJ/mol	NIST Webbook
hfs	-77.80	kJ/mol	NIST Webbook
hfus	18.07	kJ/mol	Joback Method
hsub	105.70 ± 0.70	kJ/mol	NIST Webbook
hvap	83.00 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.55		Aqueous Solubility Prediction Method
log10ws	-2.55		Estimated Solubility Method
logp	2.768		Crippen Method

mcvol	152.380	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
rinpol	1654.70		NIST Webbook
rinpol	1652.00		NIST Webbook
ripol	3187.00		NIST Webbook
tb	570.70	K	NIST Webbook
tb	341.15 ± 2.00	K	NIST Webbook
tc	870.29	K	Joback Method
tf	339.40	K	Energetics and structural properties of neutral and deprotonated phenyl carbinols
tf	339.90	K	Aqueous Solubility Prediction Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.15	J/mol×K	641.94	Joback Method
cpg	437.37	J/mol×K	832.23	Joback Method
cpg	427.56	J/mol×K	794.17	Joback Method
cpg	416.91	J/mol×K	756.11	Joback Method
cpg	405.33	J/mol×K	718.06	Joback Method
cpg	392.77	J/mol×K	680.00	Joback Method
cpg	446.39	J/mol×K	870.29	Joback Method
cps	236.80	J/mol×K	298.50	NIST Webbook
dvisc	0.0017424	Pa×s	386.10	Joback Method
dvisc	0.0006296	Pa×s	437.27	Joback Method
dvisc	0.0002816	Pa×s	488.44	Joback Method
dvisc	0.0001467	Pa×s	539.60	Joback Method
dvisc	0.0000856	Pa×s	590.77	Joback Method
dvisc	0.0065815	Pa×s	334.93	Joback Method
dvisc	0.0000544	Pa×s	641.94	Joback Method
hfust	23.00	kJ/mol	338.50	NIST Webbook
hfust	23.00	kJ/mol	338.50	NIST Webbook
hfust	23.00	kJ/mol	338.50	NIST Webbook
hsubt	104.50 ± 0.70	kJ/mol	318.00	NIST Webbook
hvapt	65.40	kJ/mol	506.00	NIST Webbook
hvapt	79.40 ± 0.70	kJ/mol	357.50	NIST Webbook
sfust	67.95	J/mol×K	338.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	570.70	K	99.70	NIST Webbook
tbrp	453.20	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Energetics and structural properties of neutral and deprotonated phenyl carbinols:	https://www.doi.org/10.1016/j.jct.2016.02.010
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume