Benzenemethanol, «alpha»-methyl-, (S)-

Other names:	(R)-(+)-1-phenylethanol
	Benzenemethanol, «alpha»-methyl-, («alpha»S)-
	Benzenemethanol, Â«alphaÂ»-methyl-, (Â«alphaÂ»S)-
Inchi:	InChI=1S/C8H10O/c1-7(9)8-5-3-2-4-6-8/h2-7,9H,1H3/t7-/m1/s1
InchiKey:	WAPNOHKVXSQRPX-SSDOTTSWSA-N
Formula:	C8H10O
SMILES:	CC(O)c1ccccc1
Mol. weight [g/mol]:	122.16
CAS:	1445-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-10.37	kJ/mol	Joback Method
hf	-129.43	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.740		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	500.86	K	Joback Method
tc	702.73	K	Joback Method
tf	252.16	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.82	J/mol×K	500.86	Joback Method
cpg	234.83	J/mol×K	534.50	Joback Method
cpg	245.20	J/mol×K	568.15	Joback Method
cpg	254.95	J/mol×K	601.79	Joback Method
cpg	264.10	J/mol×K	635.44	Joback Method
cpg	272.69	J/mol×K	669.08	Joback Method

cpg	280.74	J/mol×K	702.73	Joback Method
dvisc	0.0382650	Pa×s	252.16	Joback Method
dvisc	0.0077399	Pa×s	293.61	Joback Method
dvisc	0.0023249	Pa×s	335.06	Joback Method
dvisc	0.0009101	Pa×s	376.51	Joback Method
dvisc	0.0004291	Pa×s	417.96	Joback Method
dvisc	0.0002317	Pa×s	459.41	Joback Method
dvisc	0.0001385	Pa×s	500.86	Joback Method
rhol	1012.40	kg/m3	298.15	Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.20	K	2.70	NIST Webbook

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=C1445916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpic changes on mixing two couples of S- and R-enantiomers of benzyl-(1-phenyl-ethyl)-amine, 1-phenylethylamine, 1-phenyl-ethanol, butyric acid oxiranylmethyl ester, 4-methyl-[1,3]dioxolan-2-one, 2-chloro-methyloxirane and 3-hydroxyisobutyric acid methyl ester at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2005.10.019

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
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume