Benzyl methyl ketone

Other names:	.alpha.-phenylacetone 1-Phenylpropan-2-one 1-phenyl-2-propanone 1-phenylacetone 2-propanone, 1-phenyl- 3-phenyl-2-propanone Fenproporex-M (desamino-oxo-) NSC 9827 P2P acetone, phenyl- benzylmethylketon methyl benzyl ketone phenyl-2-propanone phenylacetone phenylmethyl methyl ketone propanone, phenyl- «alpha»-Phenylacetone
Inchi:	InChI=1S/C9H10O/c1-8(10)7-9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	QCCDLTOVEPVEJK-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC(=O)Cc1ccccc1
Mol. weight [g/mol]:	134.18
CAS:	103-79-7

Physical Properties

Property code	Value	Unit	Source
affp	842.60	kJ/mol	NIST Webbook
basg	810.80	kJ/mol	NIST Webbook
chl	-4818.80 ± 1.70	kJ/mol	NIST Webbook
chl	-4808.20 ± 1.20	kJ/mol	NIST Webbook
chl	-4818.00 ± 3.00	kJ/mol	NIST Webbook
chl	-4818.50 ± 1.70	kJ/mol	NIST Webbook
gf	8.39	kJ/mol	Joback Method
hf	-94.64	kJ/mol	NIST Webbook
hf	-94.64	kJ/mol	NIST Webbook
hfl	-162.50 ± 1.30	kJ/mol	NIST Webbook
hfl	-151.90 ± 1.70	kJ/mol	NIST Webbook

hfl	-152.30	kJ/mol	NIST Webbook
hfus	14.71	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
ie	8.98	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	9.14 ± 0.09	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	1.818		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1110.30		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1110.30		NIST Webbook
rinpol	1091.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1704.00		NIST Webbook
tb	489.70	K	NIST Webbook
tc	704.23	K	Joback Method
tf	257.80 ± 0.40	K	NIST Webbook
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.47	J/mol×K	485.87	Joback Method
cpg	246.41	J/mol×K	522.26	Joback Method
cpg	258.54	J/mol×K	558.66	Joback Method

cpg	269.91	J/mol×K	595.05	Joback Method
cpg	280.54	J/mol×K	631.45	Joback Method
cpg	290.46	J/mol×K	667.84	Joback Method
cpg	299.72	J/mol×K	704.23	Joback Method
dvisc	0.0030402	Pa×s	267.54	Joback Method
dvisc	0.0015978	Pa×s	303.93	Joback Method
dvisc	0.0009636	Pa×s	340.32	Joback Method
dvisc	0.0006407	Pa×s	376.71	Joback Method
dvisc	0.0004578	Pa×s	413.09	Joback Method
dvisc	0.0003454	Pa×s	449.48	Joback Method
dvisc	0.0002719	Pa×s	485.87	Joback Method
rhol	999.02	kg/m3	298.15	Thermodynamics of aromatic polar compound (alkanone, alkanal or alkanoate) + hydrocarbon mixtures

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamics of aromatic polar compound (alkanone, alkanal or alkanoate) + hydrocarbon mixtures:	https://www.doi.org/10.1016/j.fluid.2016.04.004
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=C103797&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase 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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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