2-Butanone, 4-phenyl-

Other names:	1-Phenyl-3-butanone
	2-Phenylethyl methyl ketone
	4-Phenylbutan-2-one
	4-phenyl-2-butanone
	4-phenyl-2-butanone (benzyl acetone)
	4-phenylbutanone
	Methyl 2-phenylethyl ketone
	Methyl phenethyl ketone
	Methyl phenylethyl ketone
	NSC 44829
	NSC 813
	Phenethyl methyl ketone
	benzylacetone
	«beta»-Phenylethyl methyl ketone
Inchi:	InChI=1S/C10H12O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-6H,7-8H2,1H3
InchiKey:	AKGGYBADQZYZPD-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CC(=O)CCc1ccccc1
Mol. weight [g/mol]:	148.20
CAS:	2550-26-7

Physical Properties

Property code	Value	Unit	Source
gf	16.81	kJ/mol	Joback Method
hf	-125.78	kJ/mol	Joback Method
hfus	17.30	kJ/mol	Joback Method
hvap	46.88	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.208		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1210.00		NIST Webbook

rinpol	1217.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1199.40		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1210.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1882.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1851.00		NIST Webbook
tb	405.00 ± 2.00	K	NIST Webbook
tb	508.20	K	NIST Webbook
tc	723.65	K	Joback Method
tf	278.81	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.20	J/mol×K	687.83	Joback Method
cpg	327.44	J/mol×K	652.02	Joback Method
cpg	315.93	J/mol×K	616.20	Joback Method
cpg	303.65	J/mol×K	580.38	Joback Method
cpg	290.55	J/mol×K	544.57	Joback Method
cpg	276.61	J/mol×K	508.75	Joback Method
cpg	348.26	J/mol×K	723.65	Joback Method
dvisc	0.0031046	Pa×s	278.81	Joback Method
dvisc	0.0002592	Pa×s	508.75	Joback Method
dvisc	0.0003313	Pa×s	470.43	Joback Method
dvisc	0.0004422	Pa×s	432.10	Joback Method
dvisc	0.0006244	Pa×s	393.78	Joback Method
dvisc	0.0009496	Pa×s	355.46	Joback Method
dvisc	0.0015984	Pa×s	317.13	Joback Method

rhol	984.74	kg/m3	298.15	Thermodynamics of aromatic polar compound (alkanone, alkanal or alkanoate) + hydrocarbon mixtures
rhol	984.74	kg/m3	298.15	Liquid Liquid Equilibria for Systems Containing 4-Phenylbutan-2-one or Benzyl Ethanoate and Selected Alkanes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	1.70	NIST Webbook
tbrp	388.00	K	1.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2550267&Units=SI
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
Liquid Liquid Equilibria for Systems Containing 4-Phenylbutan-2-one or Benzyl Ethanoate and Selected Alkanes:	https://www.doi.org/10.1021/acs.jced.6b00803
Limiting Diffusion Coefficients of Ethyl Benzoate, Benzylacetone, and Eugenol in Carbon Dioxide at Supercritical Conditions:	https://www.doi.org/10.1021/je700646e
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume