3-Buten-2-one, 4-phenyl-

Other names:	Acetocinnamone
	Benzalacetone
	Benzylideneacetone
	Methyl «beta»-styryl ketone
	Methyl styryl ketone
	2-Phenylvinyl methyl ketone
	4-Phenyl-3-buten-2-one
	4-Phenylbutenone
	1-Buten-3-one-1-phenyl
	Benzalaceton
	Styryl methyl ketone
	4-Phenylbut-3-en-2-one
	1-Phenyl-1-buten-3-one
	4-Phenyl-3-butene-2-one
	Ketone, methyl styryl
	Methyl 2-phenylvinyl ketone
	NSC 5605
Inchi:	InChI=1S/C10H10O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-8H,1H3
InchiKey:	BWHOZHOGCMHOBV-UHFFFAOYSA-N
Formula:	C10H10O
SMILES:	CC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	122-57-6

Physical Properties

Property code	Value	Unit	Source
chl	-5282.30	kJ/mol	NIST Webbook
chs	-5262.20	kJ/mol	NIST Webbook
gf	97.03	kJ/mol	Joback Method
hf	-48.10 ± 3.80	kJ/mol	NIST Webbook
hfs	-102.00	kJ/mol	NIST Webbook
hfus	17.50	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.80	eV	NIST Webbook

log10ws	-2.41		Crippen Method
logp	2.289		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1346.20		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1337.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2095.00		NIST Webbook
tb	534.20	K	NIST Webbook
tc	738.22	K	Joback Method
tf	314.00 ± 3.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.13	J/mol×K	738.22	Joback Method
cpg	316.88	J/mol×K	700.67	Joback Method
cpg	306.90	J/mol×K	663.11	Joback Method
cpg	296.15	J/mol×K	625.56	Joback Method
cpg	284.57	J/mol×K	588.01	Joback Method
cpg	272.10	J/mol×K	550.46	Joback Method
cpg	258.70	J/mol×K	512.91	Joback Method
dvisc	0.0028529	Pa×s	273.73	Joback Method
dvisc	0.0002186	Pa×s	512.91	Joback Method
dvisc	0.0002801	Pa×s	473.05	Joback Method
dvisc	0.0003755	Pa×s	433.18	Joback Method
dvisc	0.0005344	Pa×s	393.32	Joback Method
dvisc	0.0008235	Pa×s	353.46	Joback Method
dvisc	0.0014163	Pa×s	313.59	Joback Method
hvapt	58.50	kJ/mol	444.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume