3-Buten-2-one, 4-phenyl-, (E)-

Other names:	trans-Benzalacetone
	trans-Benzylidenacetone
	trans-Benzylideneacetone
	Methyl trans-styryl ketone
	trans-4-Phenyl-3-butene-2-one
	TPBO
	trans-4-Phenyl-3-buten-2-one
	(3E)-4-Phenyl-3-buten-2-one
	(E)-1-Buten-3-one, 1-phenyl
	(E)-4-Phenylbut-3-en-2-one
	trans-4-phenylbut-3-en-2-one
Inchi:	InChI=1S/C10H10O/c1-9(11)7-8-10-5-3-2-4-6-10/h2-8H,1H3/b8-7+
InchiKey:	BWHOZHOGCMHOBV-BQYQJAHWSA-N
Formula:	C10H10O
SMILES:	CC(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	1896-62-4

Physical Properties

Property code	Value	Unit	Source
gf	97.03	kJ/mol	Joback Method
hf	-8.56	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	46.83	kJ/mol	Joback Method
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	1323.00		NIST Webbook
rinpol	1330.00		NIST Webbook
ripol	2032.00		NIST Webbook
tb	535.20	K	NIST Webbook
tc	738.22	K	Joback Method
tf	273.73	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1896624&Units=SI

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
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